Molecular QCA and the limits of binary switching logic

Craig S. Lent
University of Notre Dame

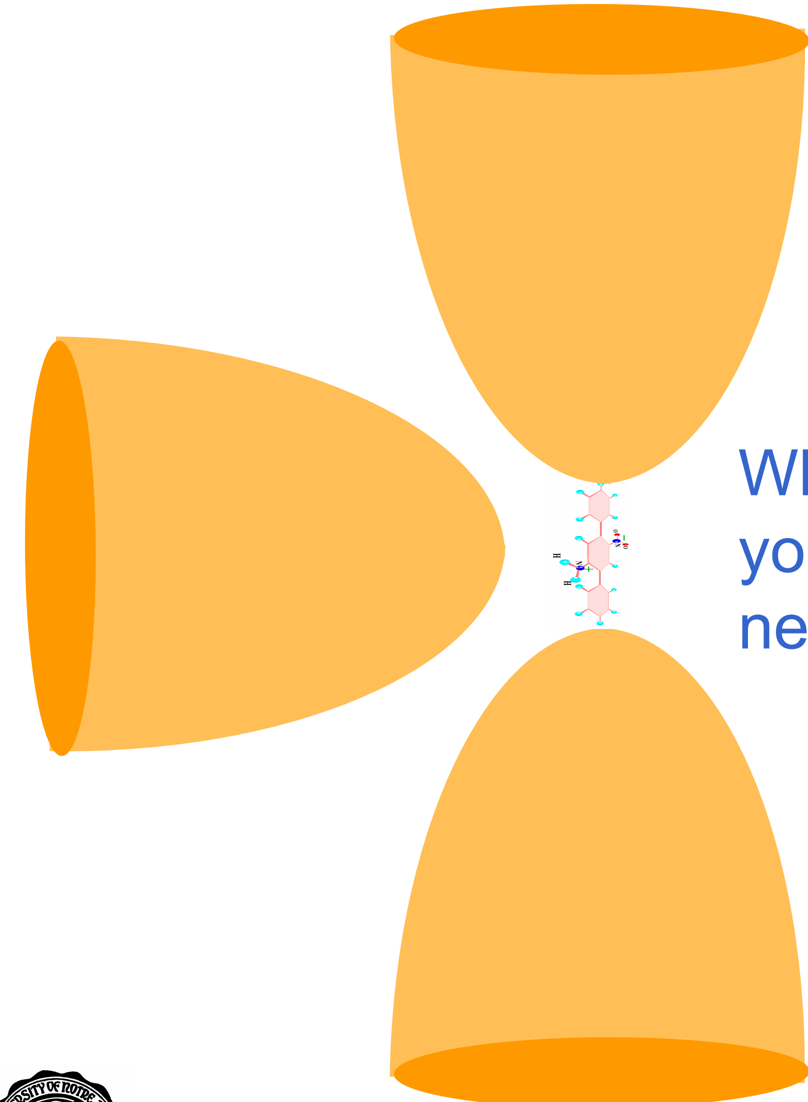
Collaborators: Peter Kogge, Mike Niemier, Greg Snider, Patrick Fay, Marya Lieberman, Thomas Fehlner, Alex Kandel

Supported by NSF, State of Indiana

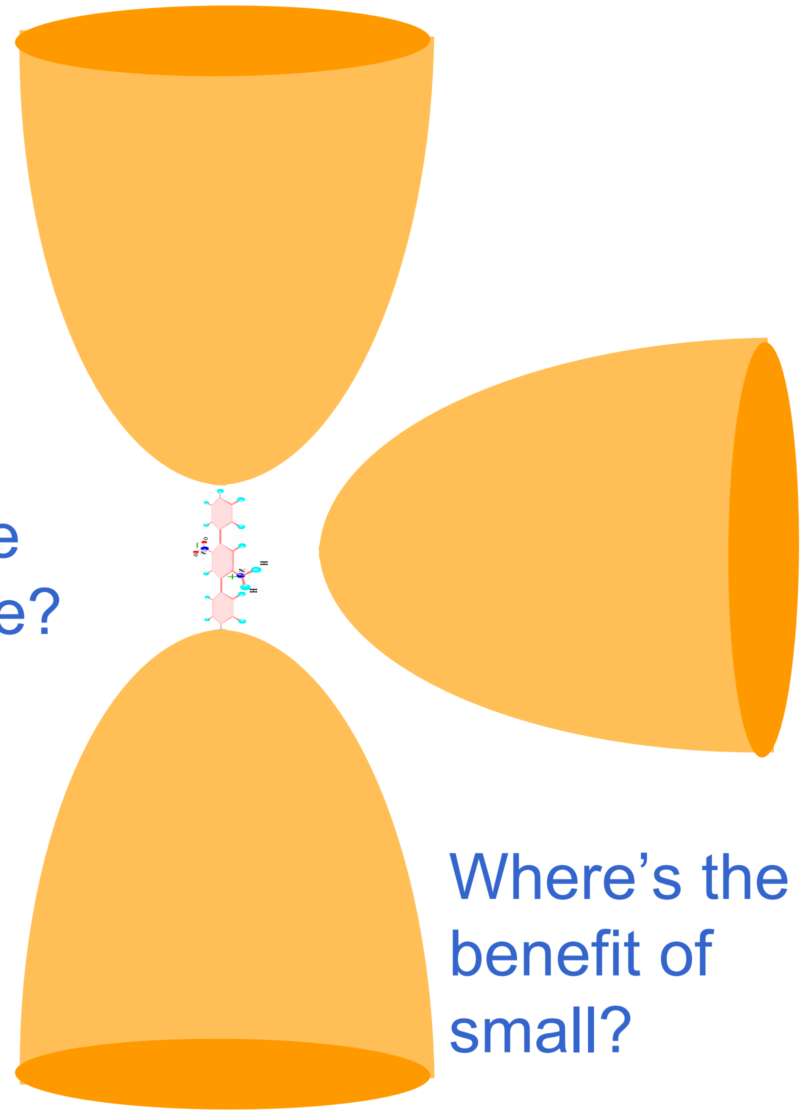
The Dream of Molecular Transistors

Why don't we keep on shrinking transistors until they are each a single molecule?

Molecular Transistors

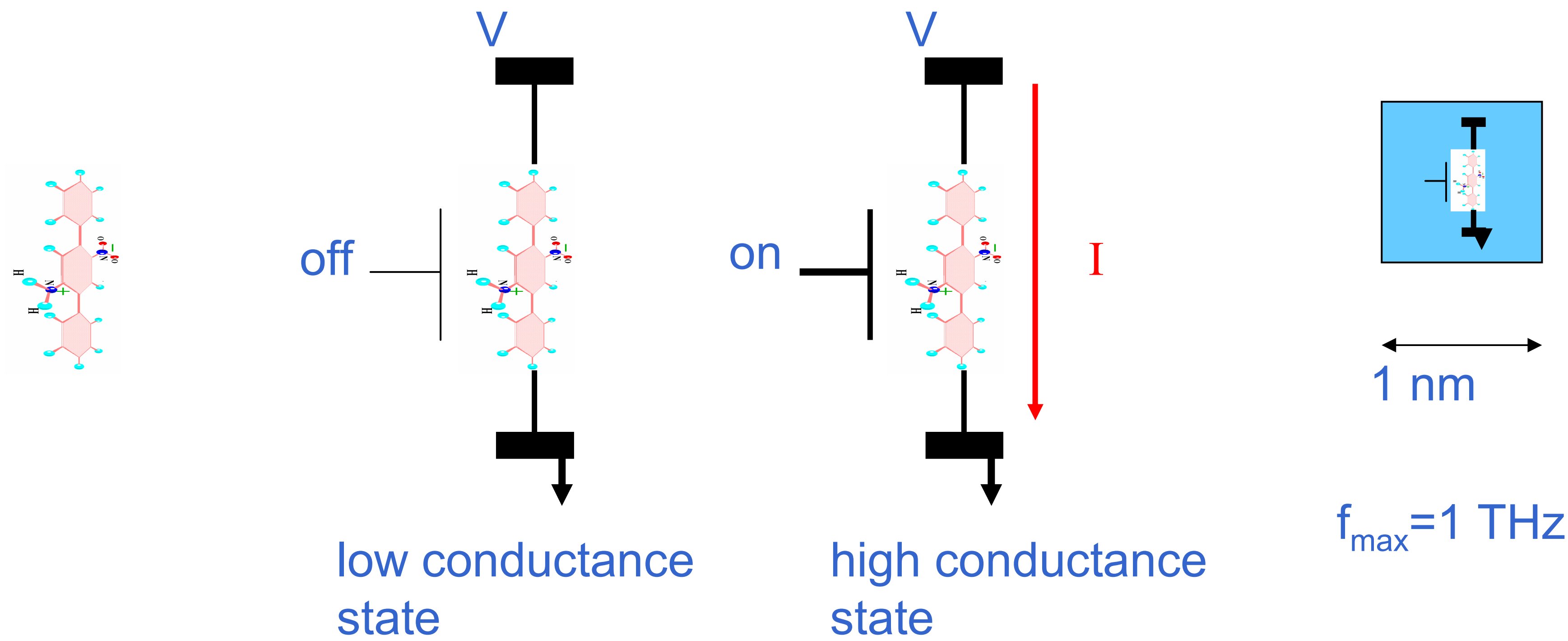


Where do you put the next device?



Where's the benefit of small?

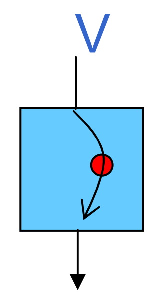
Dream molecular transistors



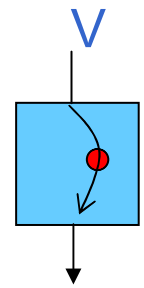
Molecular densities: 1nm x 1nm → $10^{14}/cm^2$

Transistors at molecular densities

Suppose in each clock cycle a *single* electron moves from power supply (1V) to ground.



Transistors at molecular densities



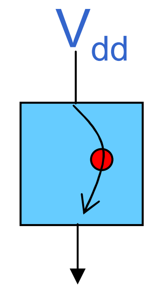
Suppose in each clock cycle a *single* electron moves from power supply (1V) to ground.

Power dissipation (Watts/cm^2)

Frequency (Hz)	10^{14} devices/cm^2	10^{13} devices/cm^2	10^{12} devices/cm^2	10^{11} devices/cm^2
10^{12}	16,000,000	1,600,000	160,000	16,000
10^{11}	1,600,000	160,000	16,000	1,600
10^{10}	160,000	16,000	1,600	160
10^{9}	16,000	1600	160	16
10^{8}	1600	160	16	1.6
10^{7}	160	16	1.6	0.16
10^{6}	16	1.6	0.16	0.016

ITRS roadmap:
7nm gate length, 10^9 logic transistors/cm^2 @ 3x10^{10} Hz for 2016

Transistors at molecular densities



Suppose in each clock cycle a *single* electron moves from power supply (1V) to ground.

Power dissipation (Watts/cm^2)

Frequency (Hz)	10^{14} devices/cm^2	10^{13} devices/cm^2	10^{12} devices/cm^2	10^{11} devices/cm^2
10^{12}	16,000,000	1,600,000	160,000	16,000
10^{11}	1,600,000	160,000	16,000	1,600
10^{10}	160,000	16,000	1,600	160
10^{9}	16,000	1600	160	16
10^{8}	1600	160	16	1.6
10^{7}	160	16	1.6	0.16
10^{6}	16	1.6	0.16	0.016

ITRS roadmap:
7nm gate length, 10^9 logic transistors/cm^2 @ 3×10^{10} Hz for 2016

The Dream of Molecular Transistors

Molecular electronics requirements

1) Low power dissipation
2) Real power gain
3) Robustness to disorder

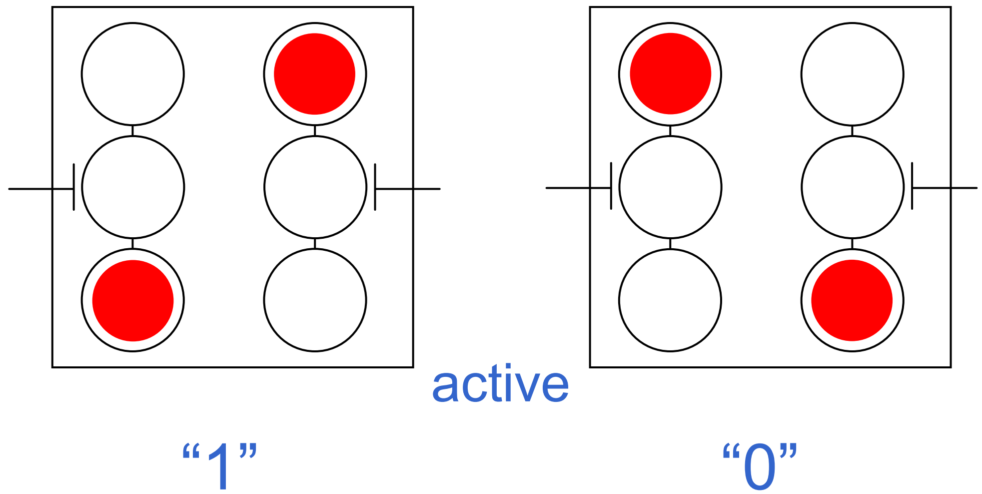
Benefit: functional densities at molecular scale

Outline

- Introduction
- QCA paradigm
- Implementations
  - Metal-dot QCA
  - Molecular QCA
- Energy flow in QCA
  - Power gain
  - Power dissipation and erasure
  - Bennett clocking

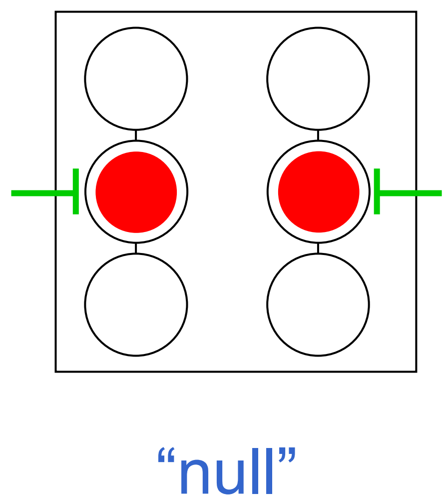
Quantum-dot cellular automata

Represent binary information by charge configuration of cell.



QCA cell

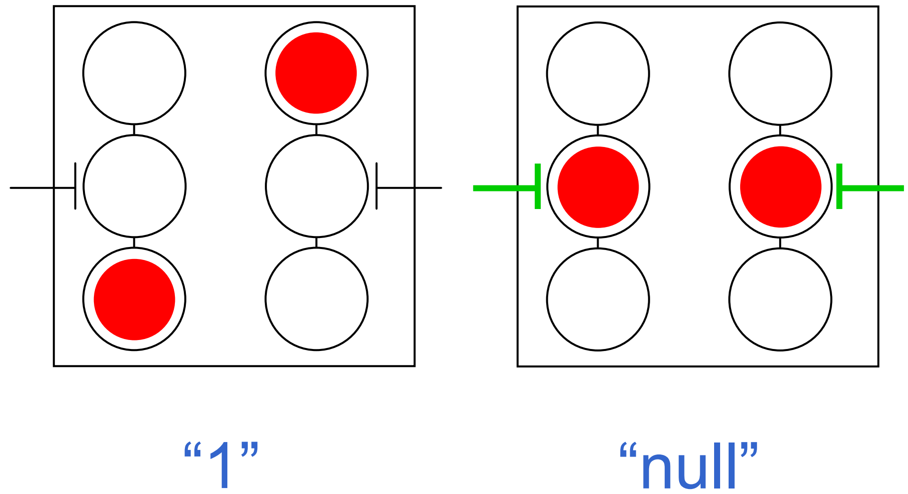
- Dots localize charge
- Two mobile charges
- Tunneling between dots
- Clock signal varies relative energies of “active” and “null” dots



Clock need not separately contact each cell.

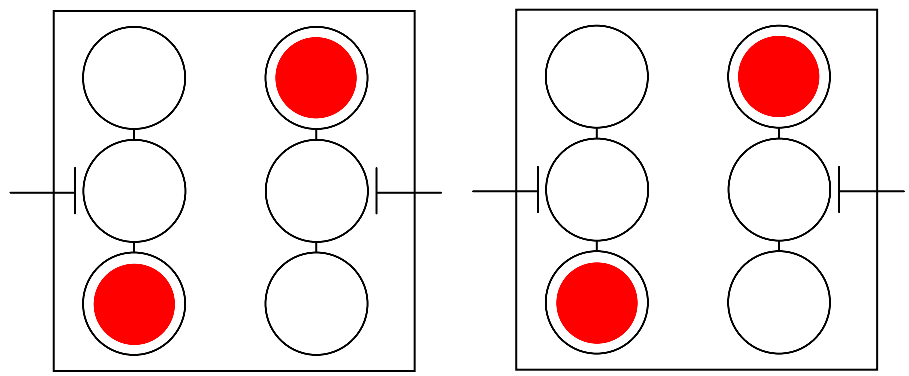
Quantum-dot cellular automata

Neighboring cells tend to align in the same state.



Quantum-dot cellular automata

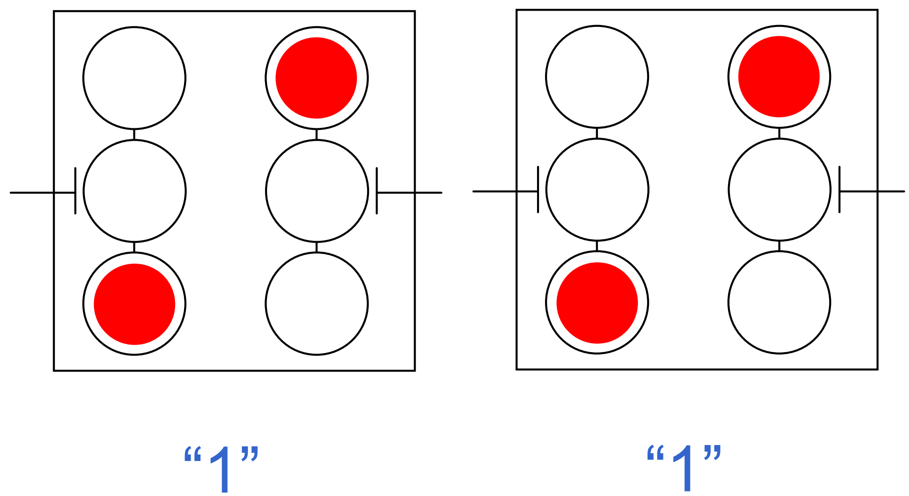
Neighboring cells tend to align in the same state.



"1" "1"

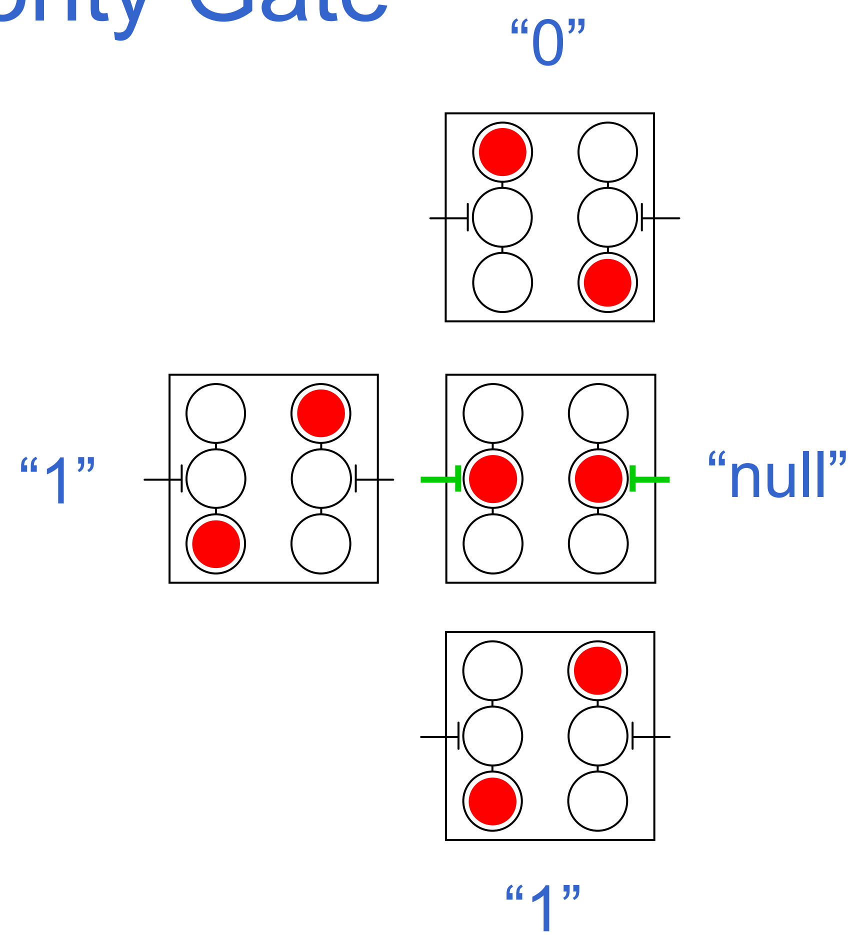
Quantum-dot cellular automata

Neighboring cells tend to align in the same state.

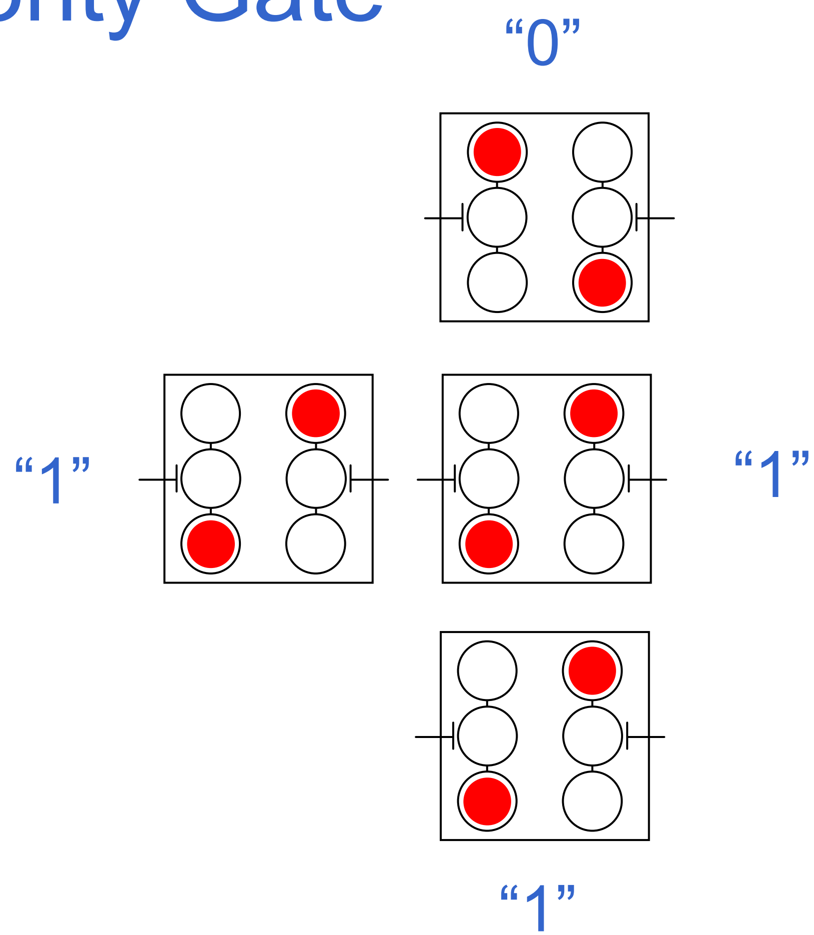


This is the COPY operation.

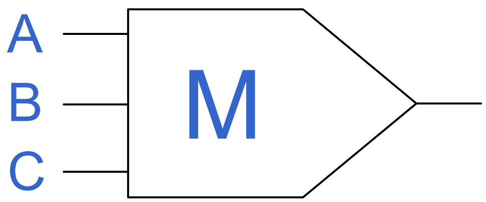
Majority Gate

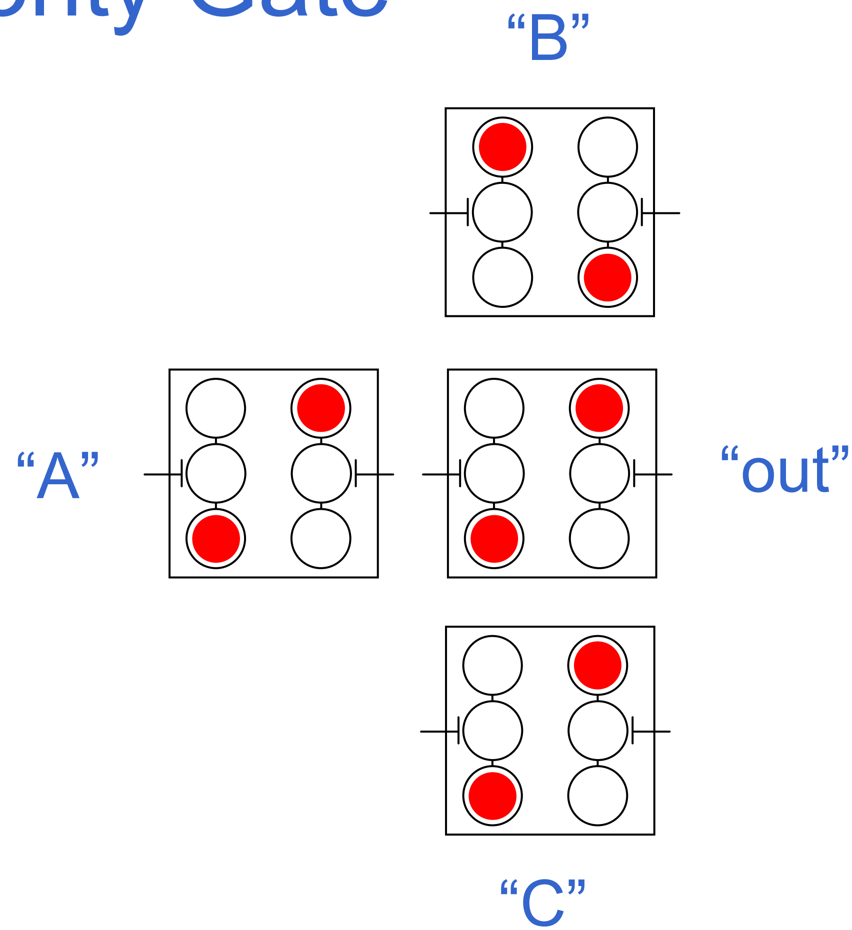


Majority Gate



Majority Gate

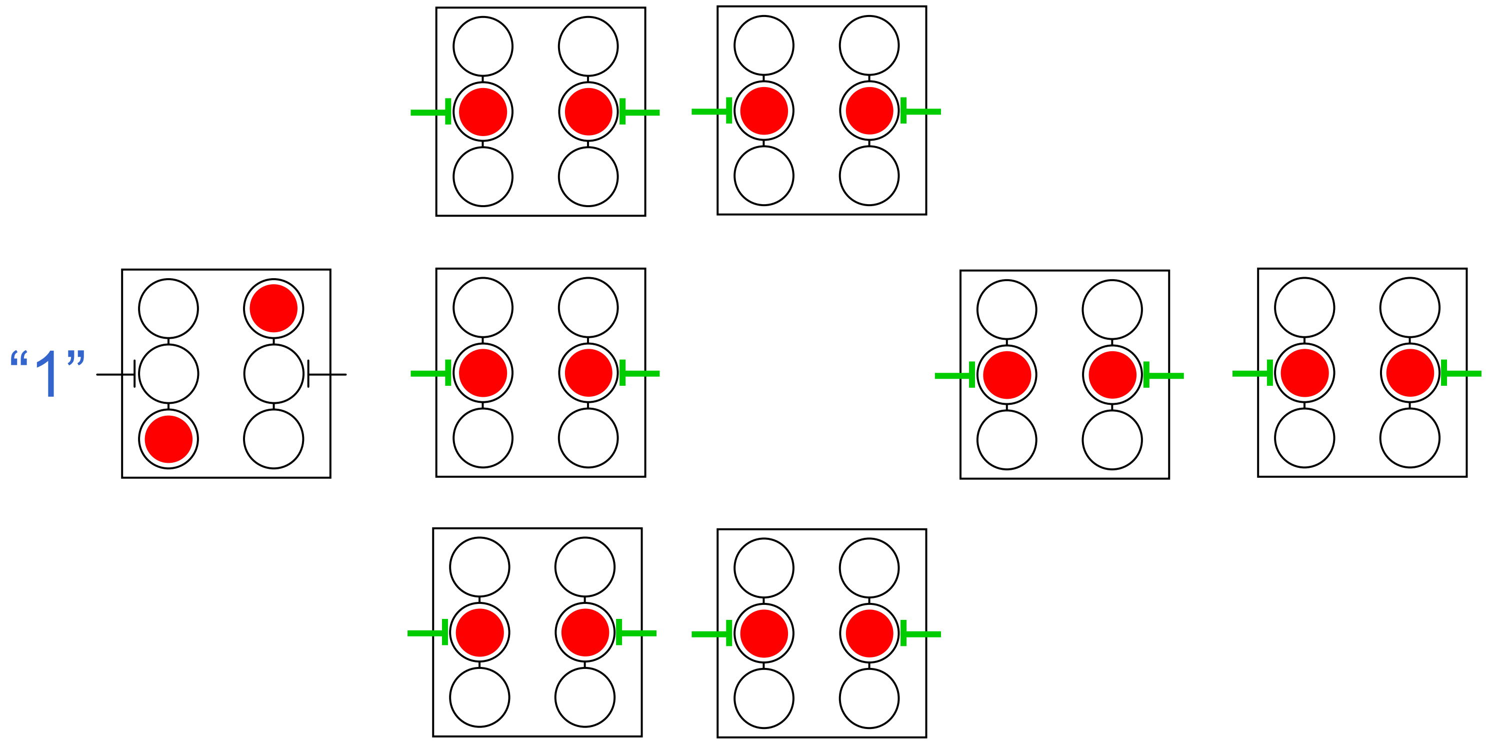




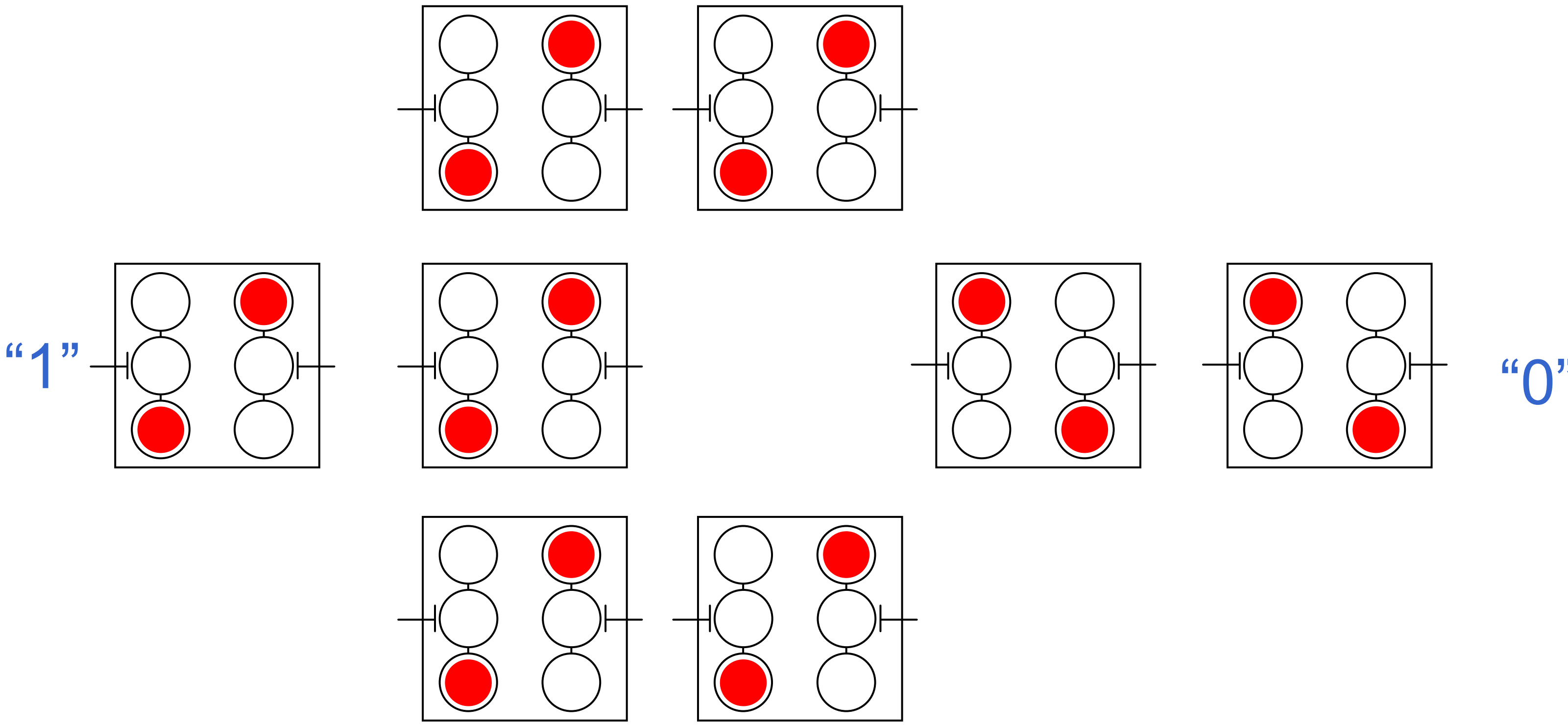
	A	B	C	Output
AND gate	0	0	0	0
AND gate	0	0	1	0
AND gate	0	1	1	1
AND gate	0	1	0	0
OR gate	1	1	0	1
OR gate	1	1	1	1
OR gate	1	0	1	1
OR gate	1	0	0	0

Three input majority gate can function as programmable 2-input AND/OR gate.

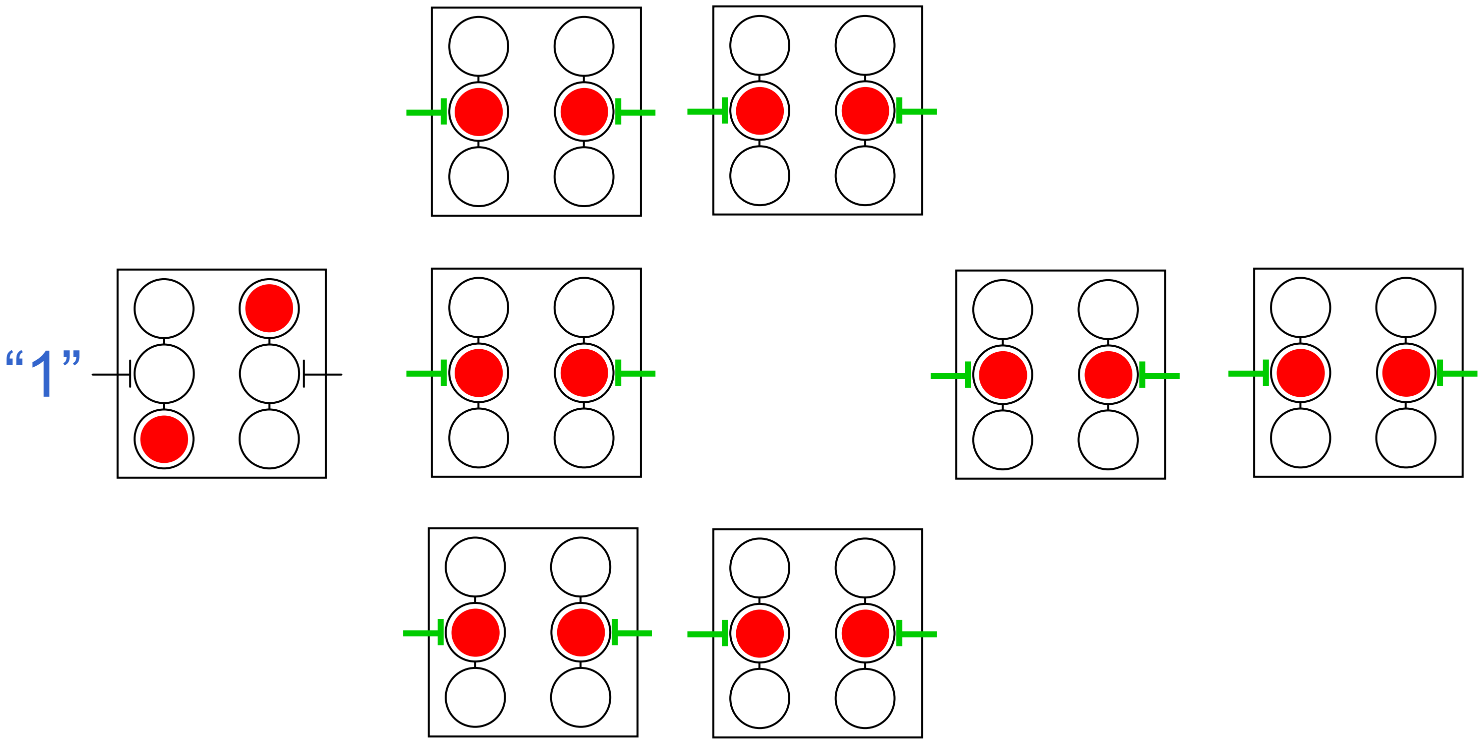
Inverter Gate



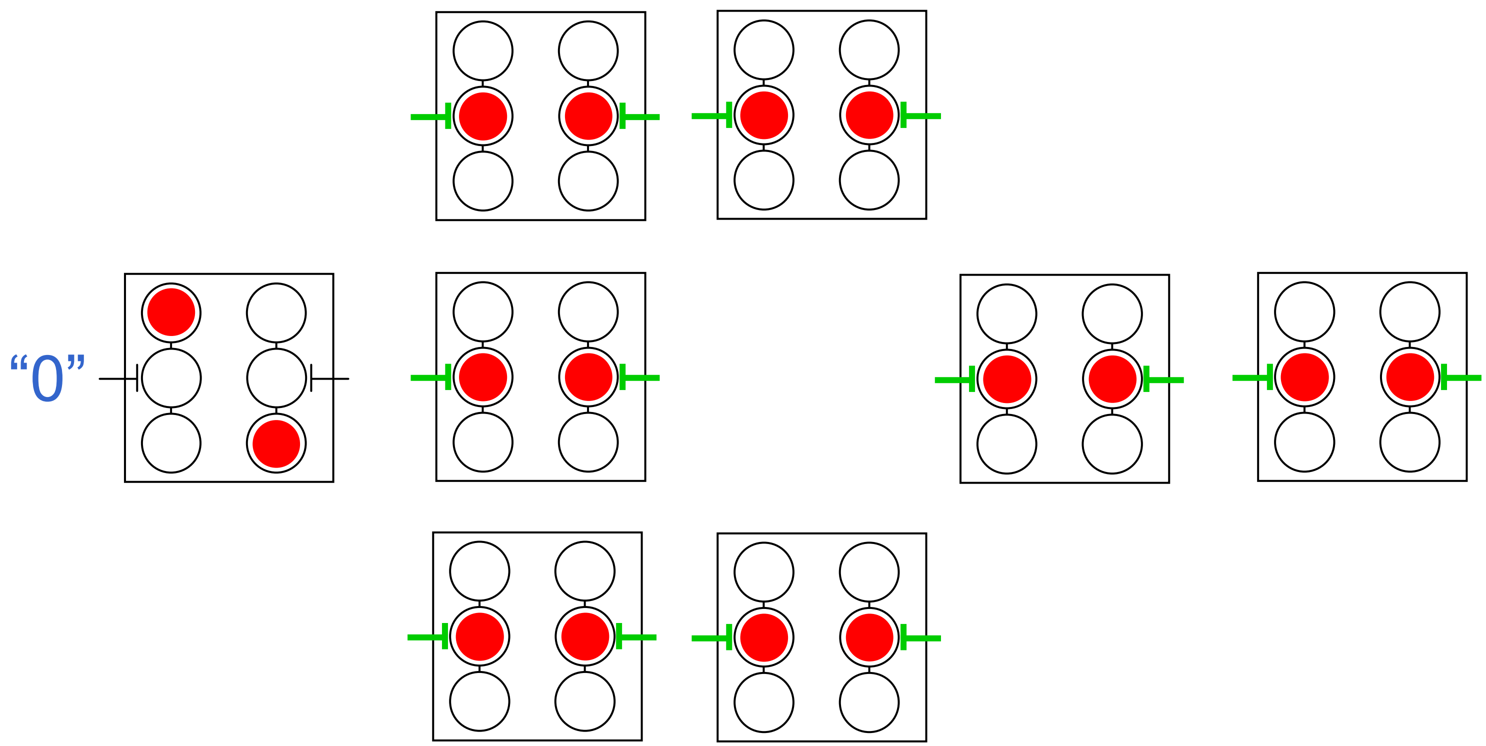
Inverter Gate



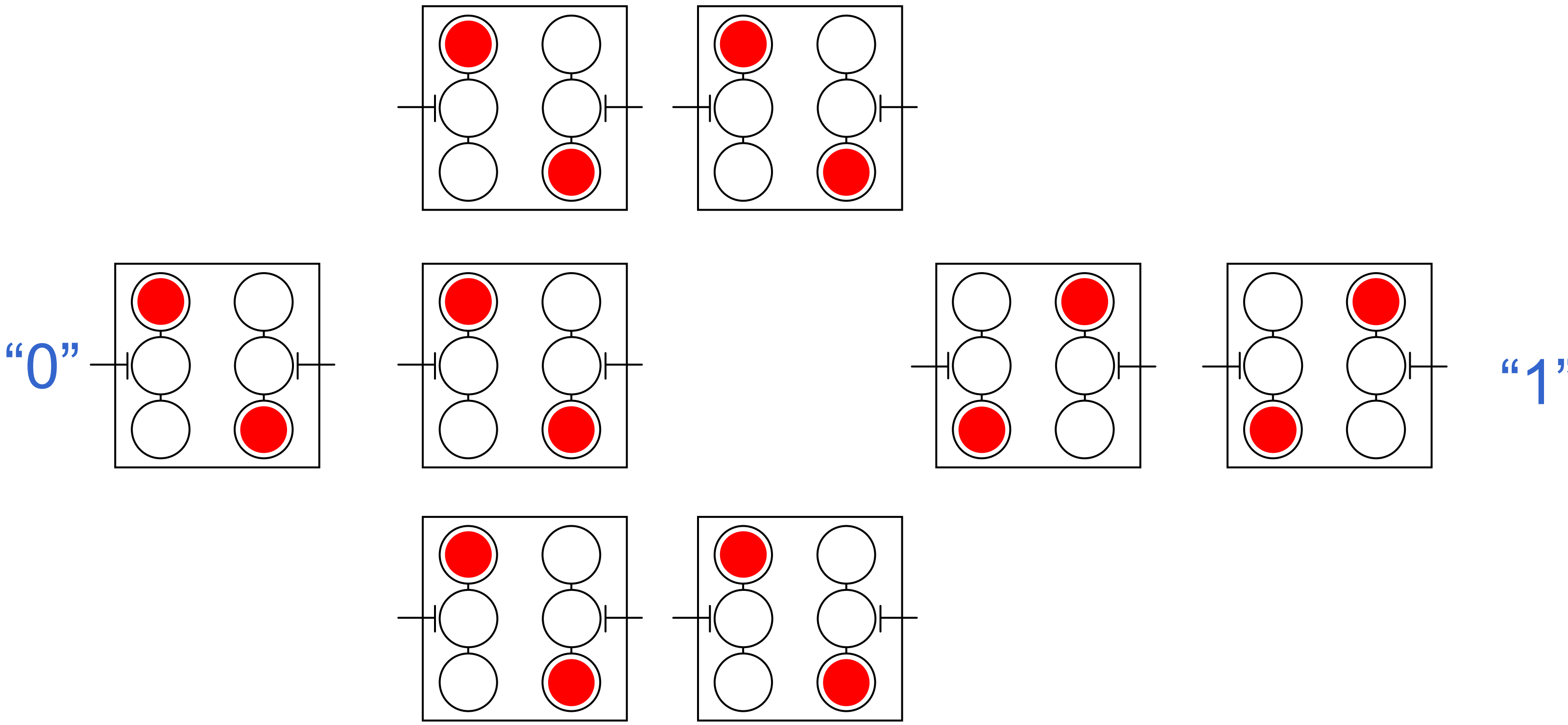
Inverter Gate



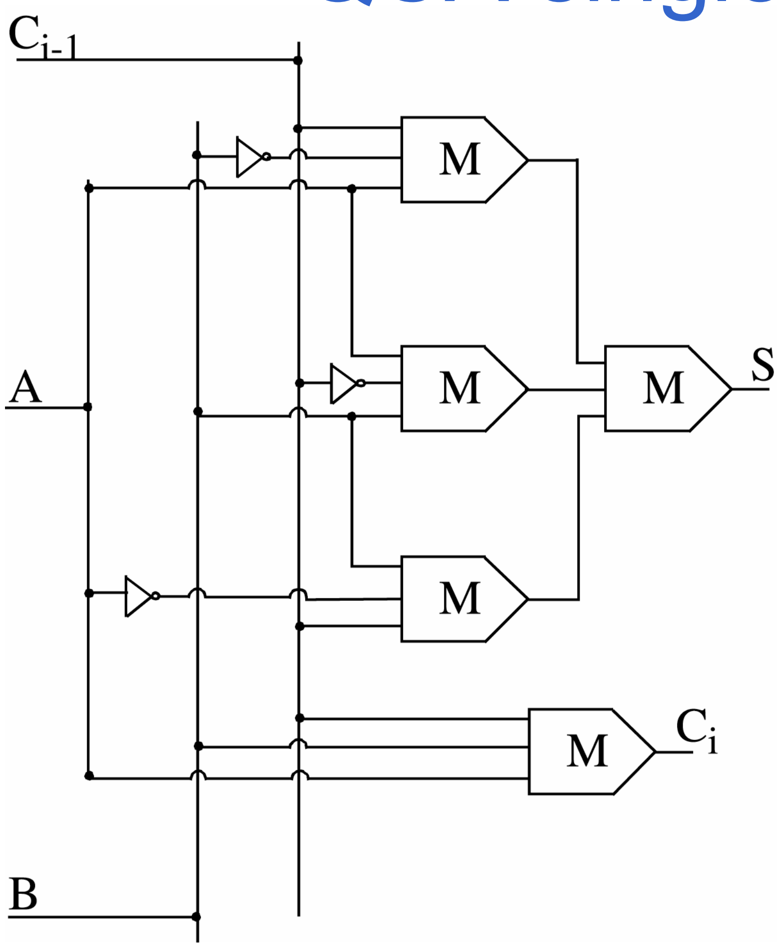
Inverter Gate

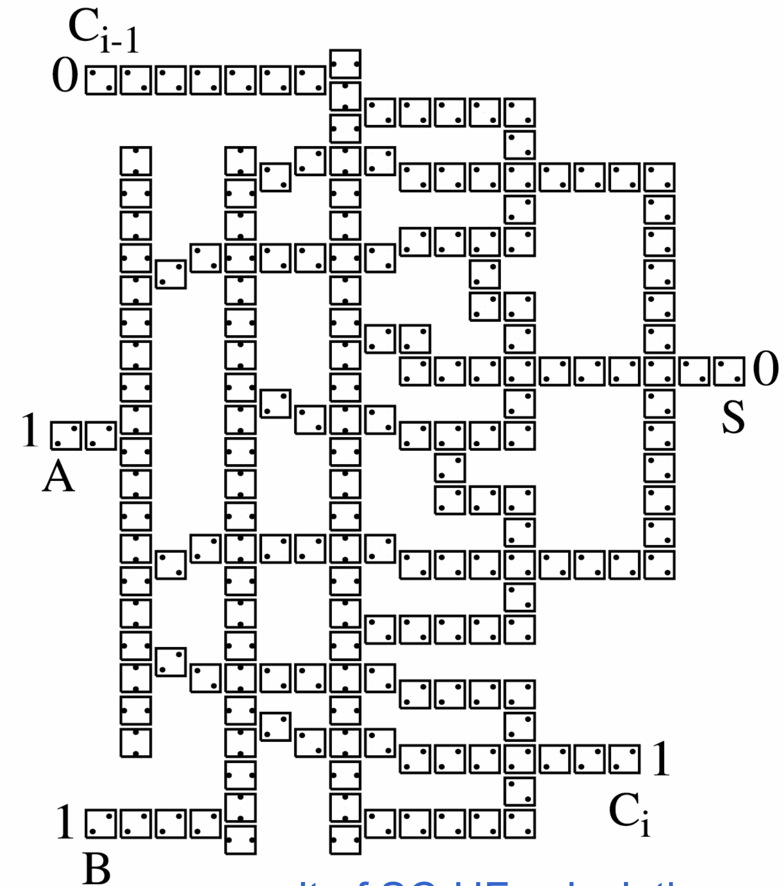


Inverter Gate



QCA single-bit full adder

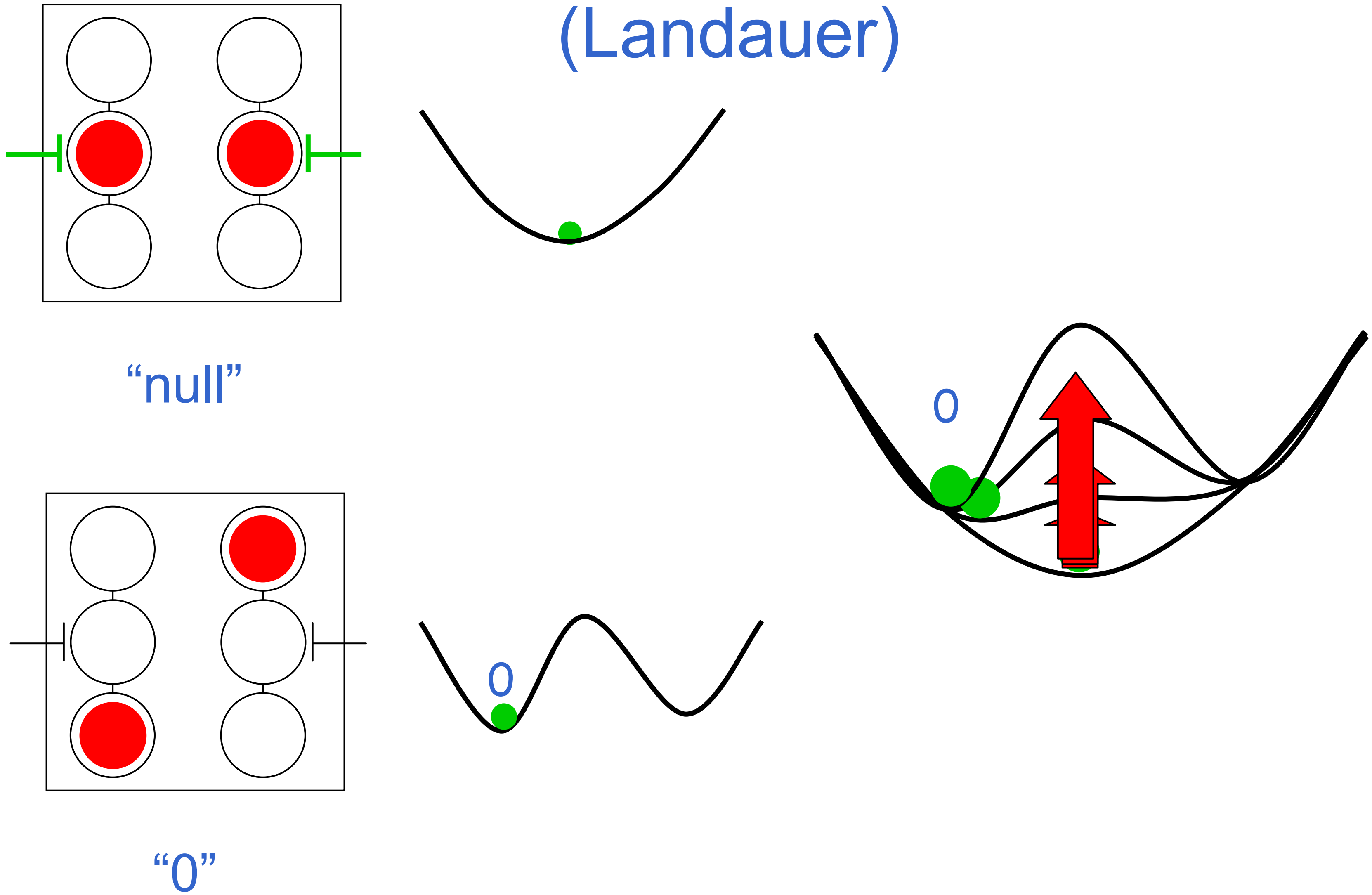




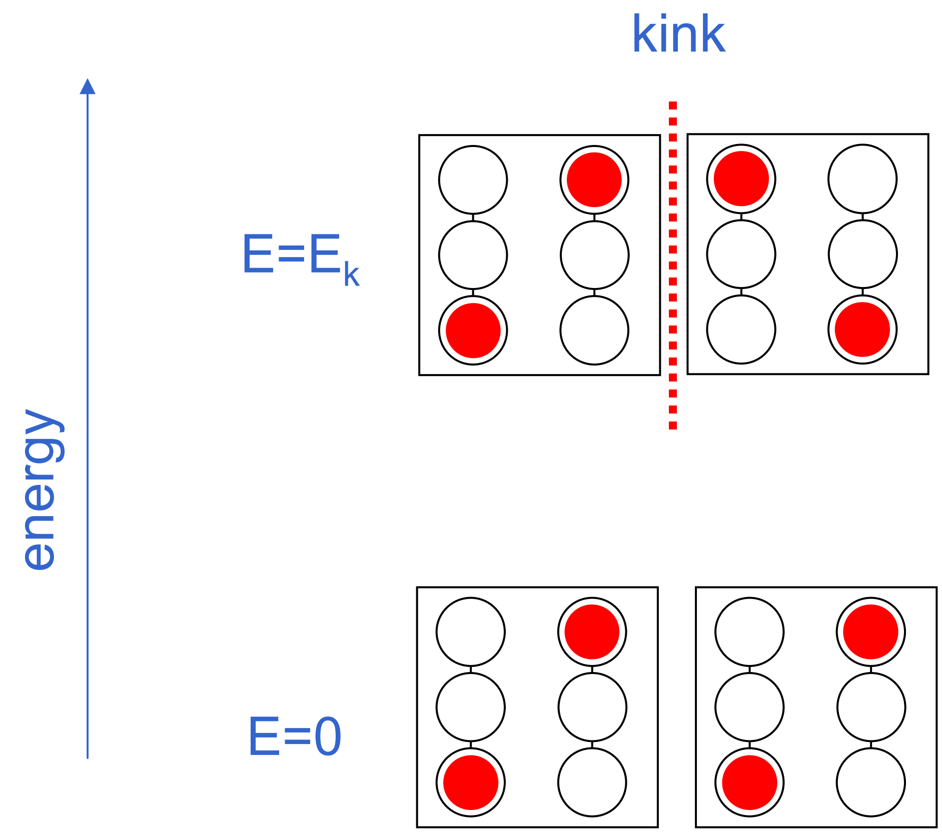
result of SC-HF calculation
with site model

Hierarchical layout and design are possible.

Adiabatic computing (Landauer)

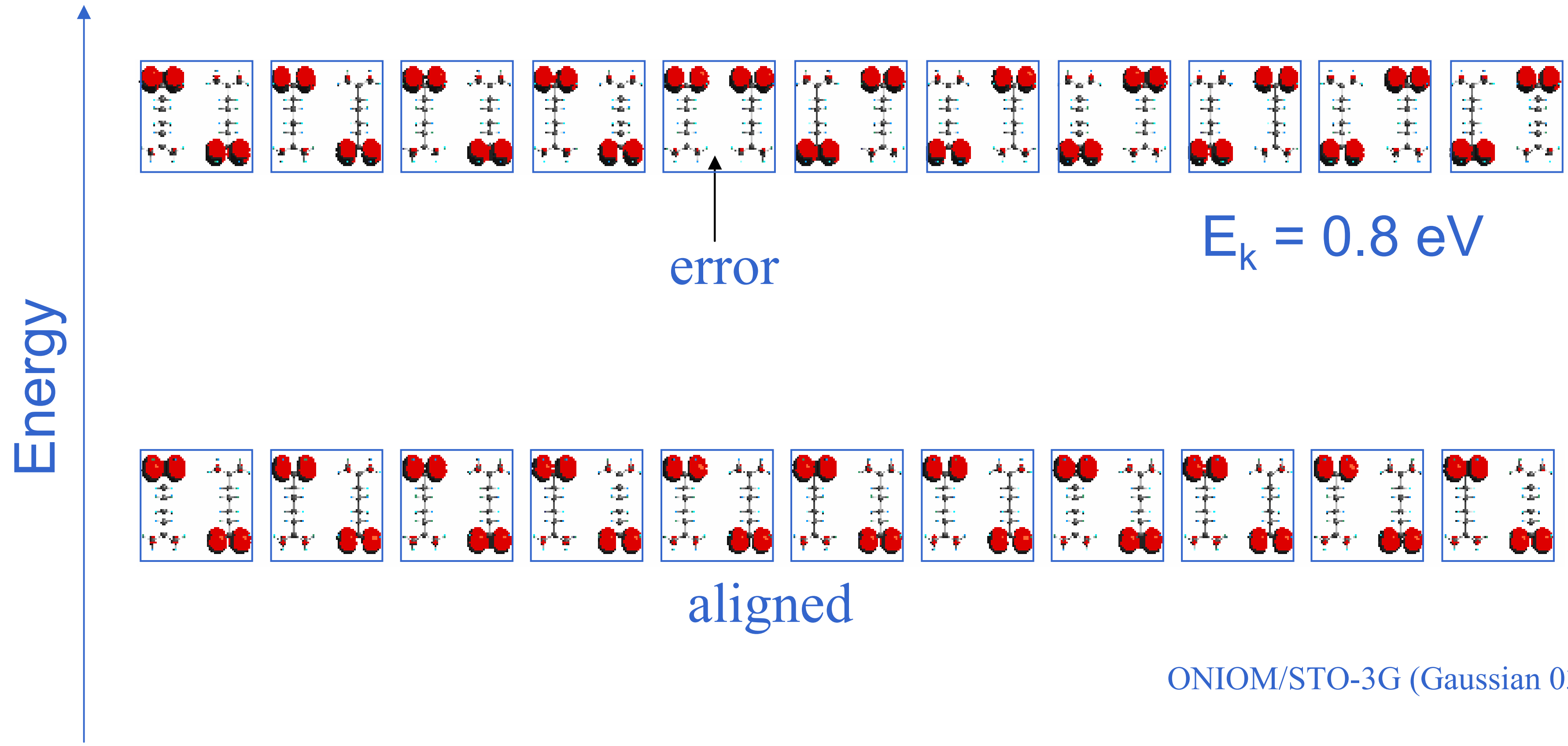


Characteristic energy



We would like "kink energy" $E_k > k_BT$.

Molecular Wire

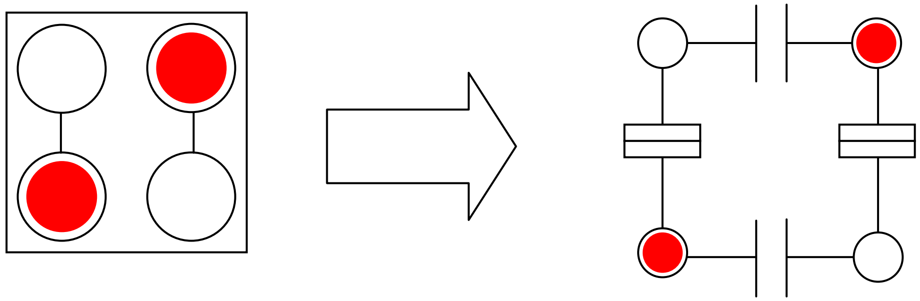


ONIOM/STO-3G (Gaussian 03)

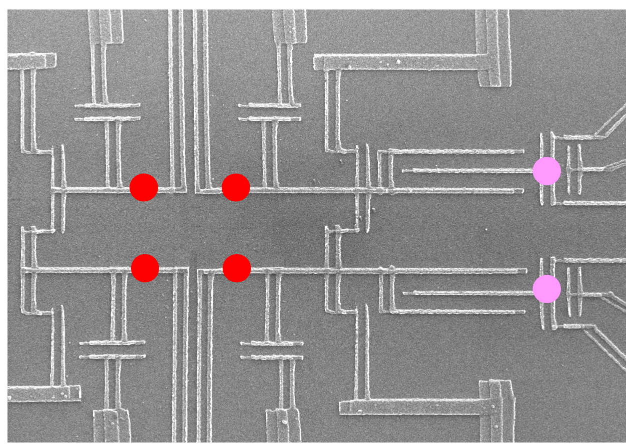
Outline

- Introduction
- QCA paradigm
- Implementations
  - Metal-dot QCA
  - Molecular QCA
- Energy flow in QCA
  - Power gain
  - Power dissipation and erasure
  - Bennett clocking

QCA devices exist



Metal-dot QCA implementation



Al/AlO_x on SiO_2

electrometers

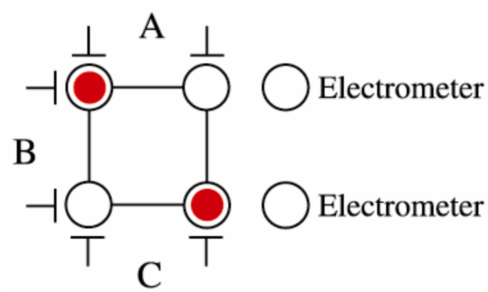
“dot” = metal island

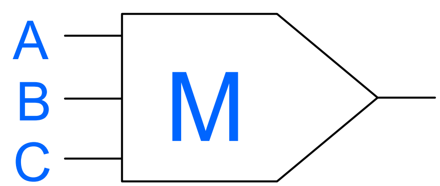
70 mK

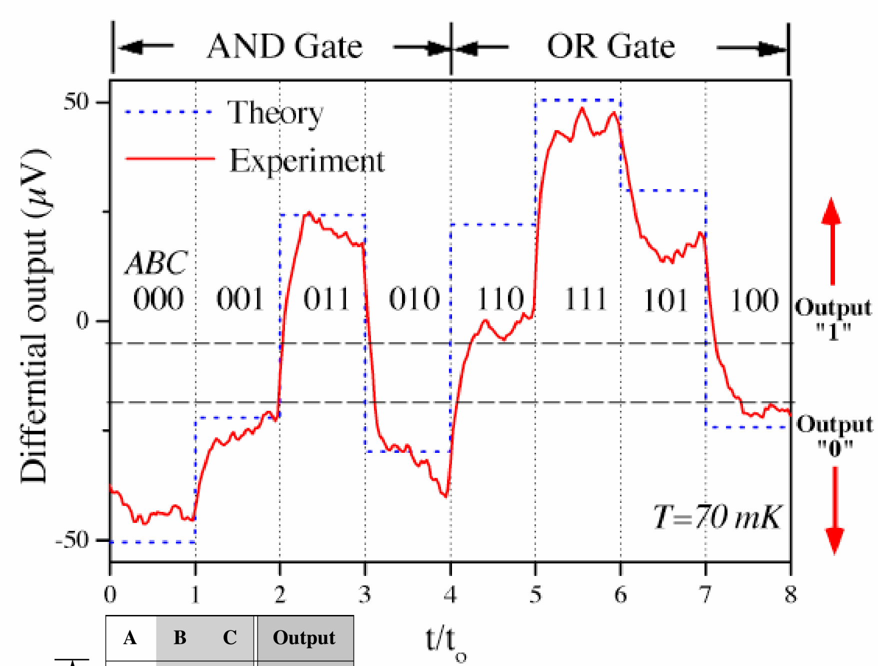
Greg Snider, Alexei Orlov, and Gary Bernstein

Metal-dot QCA cells and devices

- Majority Gate



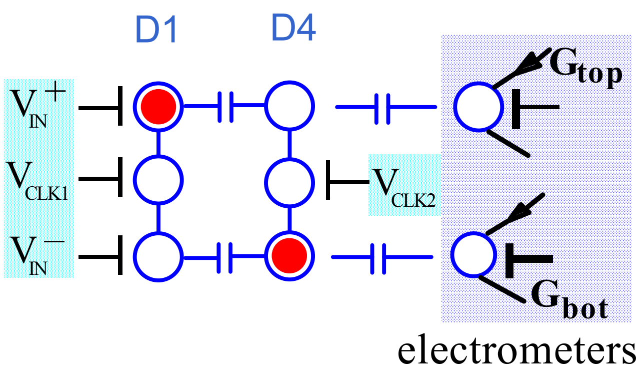


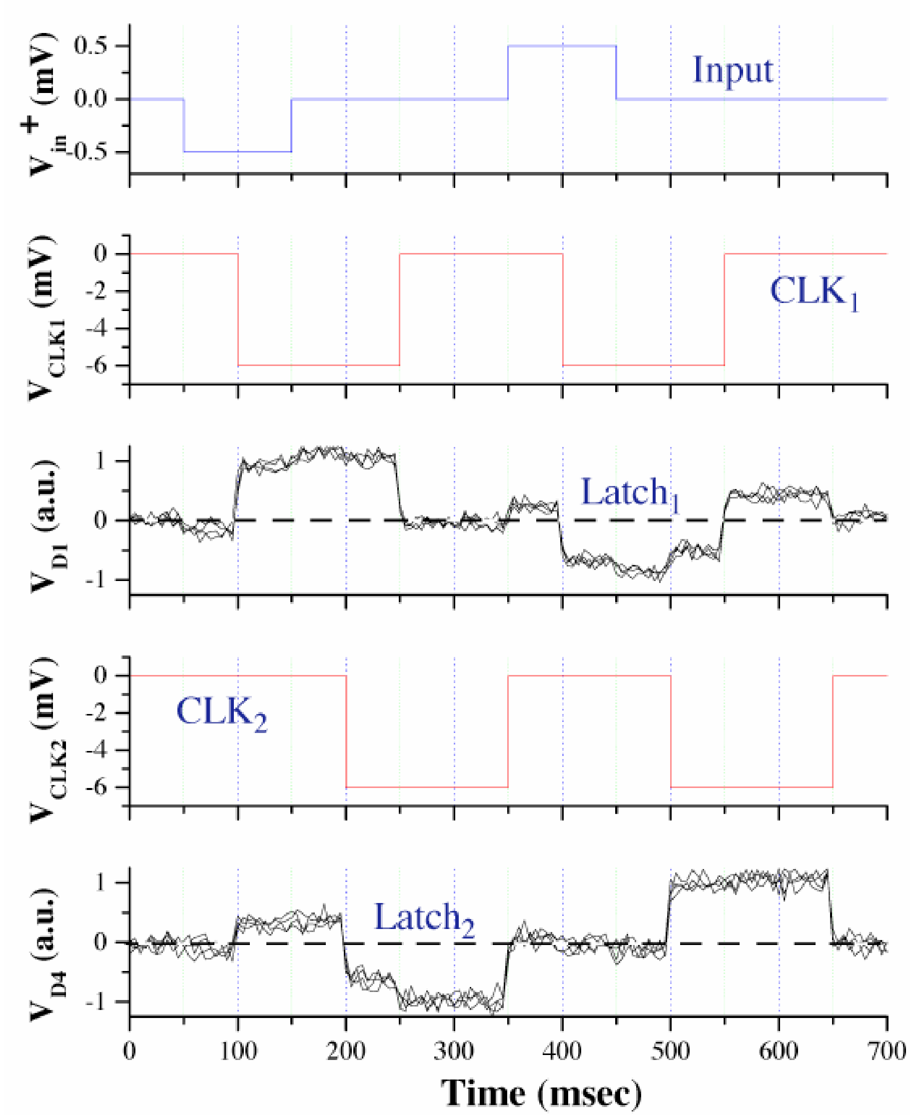


	A	B	C	Output
AND gate	0	0	0	0
	0	0	1	0
	0	1	1	1
	0	1	0	0
OR gate	1	1	0	1
	1	1	1	1
	1	0	1	1
	1	0	0	0

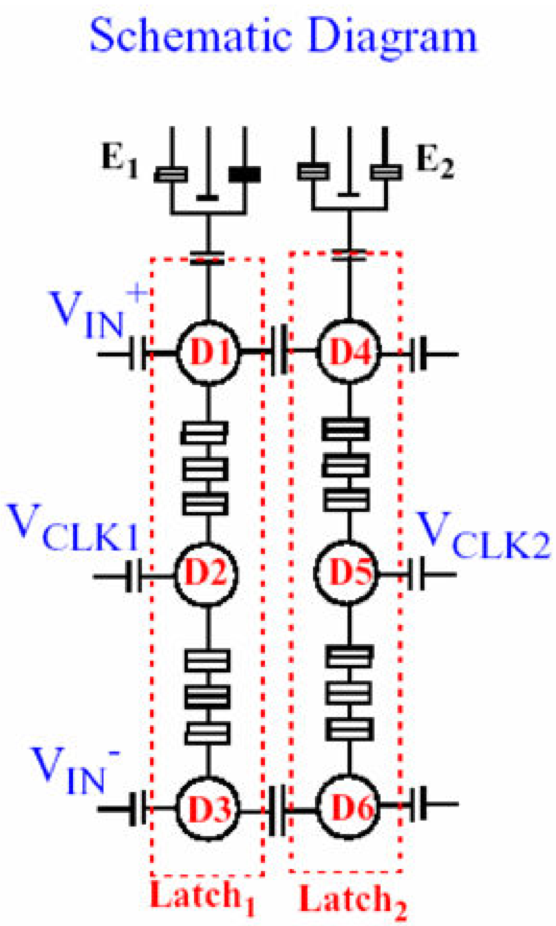
Amlani, A. Orlov, G. Toth, G. H. Bernstein, C. S. Lent, G. L. Snider, *Science* **284**, pp. 289-291 (1999).

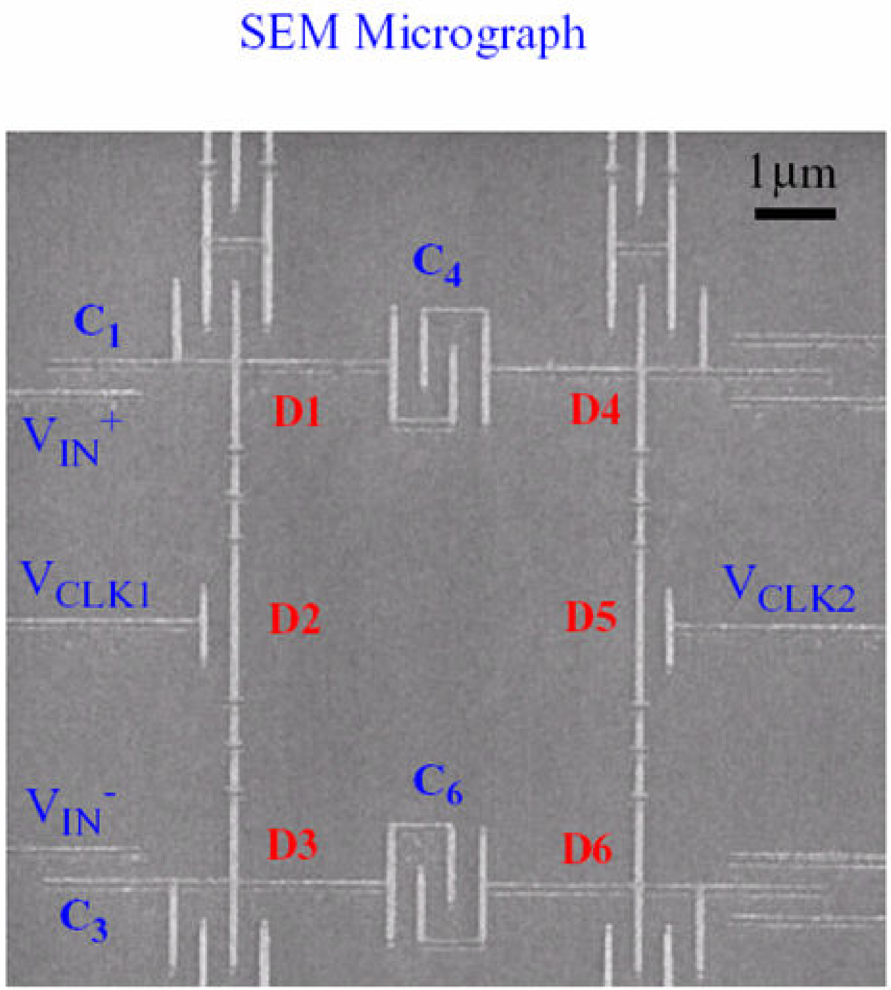
QCA Shift Register





QCA Shift Register



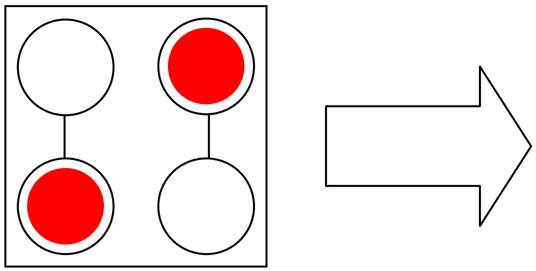


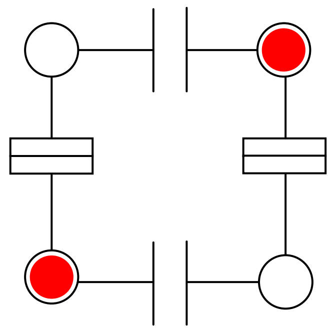
Metal-dot QCA devices exist

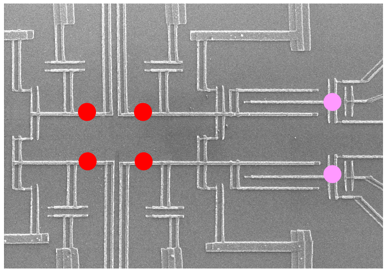
- Single electron analogue of molecular QCA
- Gates and circuits:
  - Wires
  - Shift registers
  - Fan-out
  - Power gain demonstrated
  - AND, OR, Majority gates
- Work underway to raise operating temperatures

From metal-dot to molecular QCA

Metal tunnel junctions

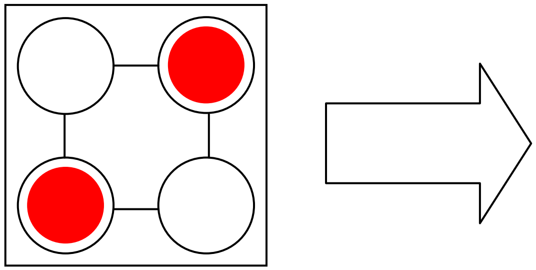


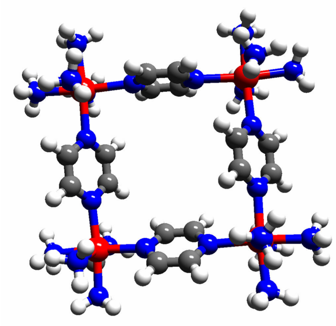




"dot" = metal island

70 mK





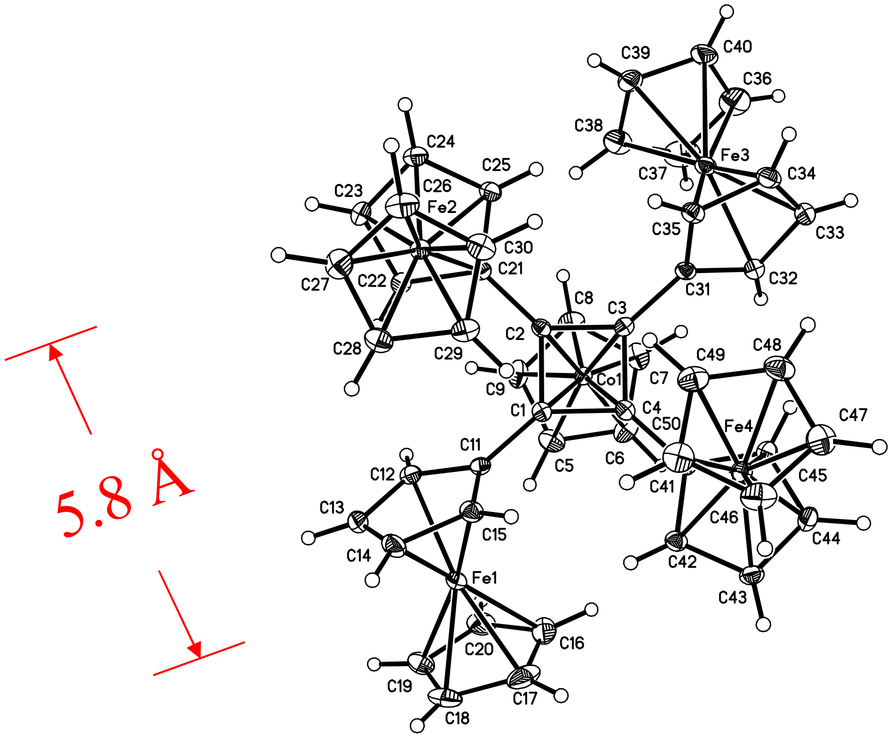
"dot" = redox center

Mixed valence compounds

room temperature+

Key strategy: use *nonbonding* orbitals (π or d) to act as dots.

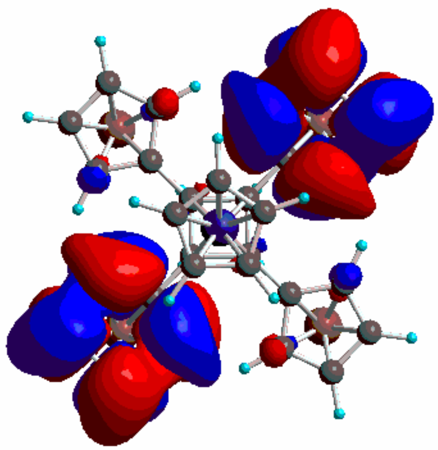
4-dot molecule



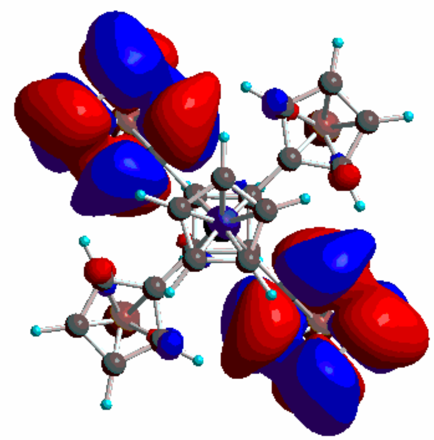
Fehlner *et al*
(Notre Dame chemistry group)
Journal of American Chemical Society
125:7522, 2003

Each ferrocene acts as a quantum dot, the Co group connects 4 dots.

Bistable configurations



"0"

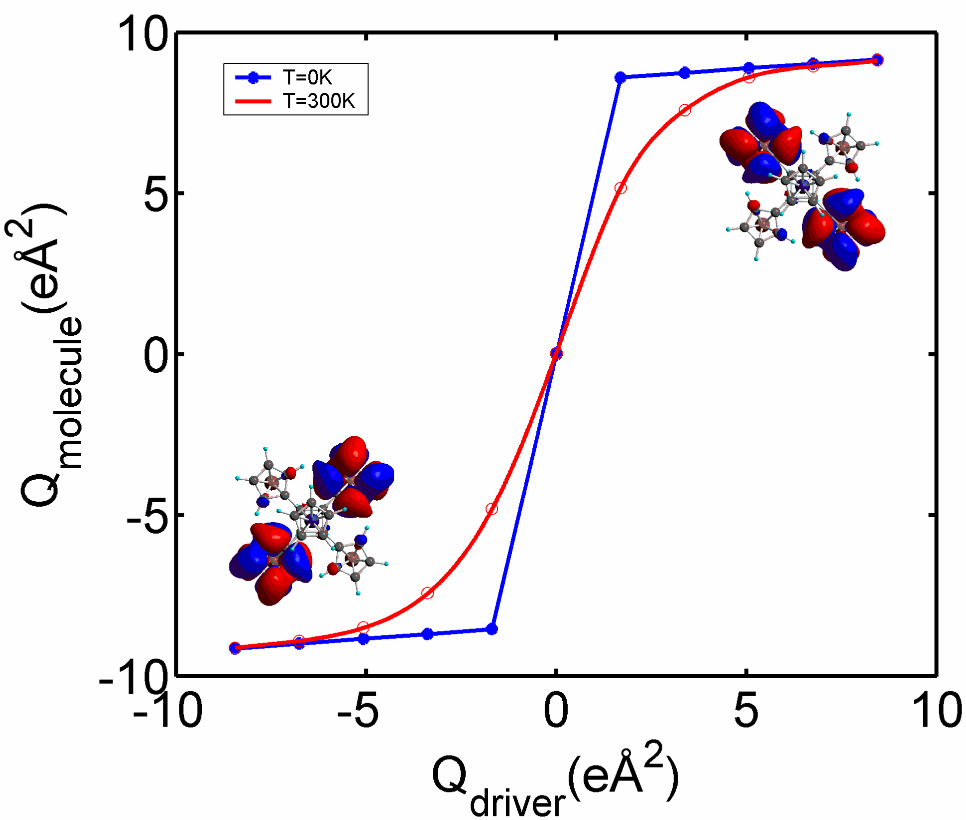


"1"

Fehlner *et al*
(Notre Dame chemistry group)
Journal of American Chemical Society
125:7522, 2003

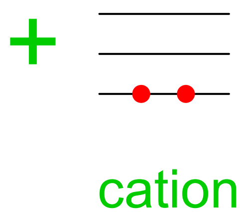
Guassian-98 UHF/STO-3G/LANL2DZ

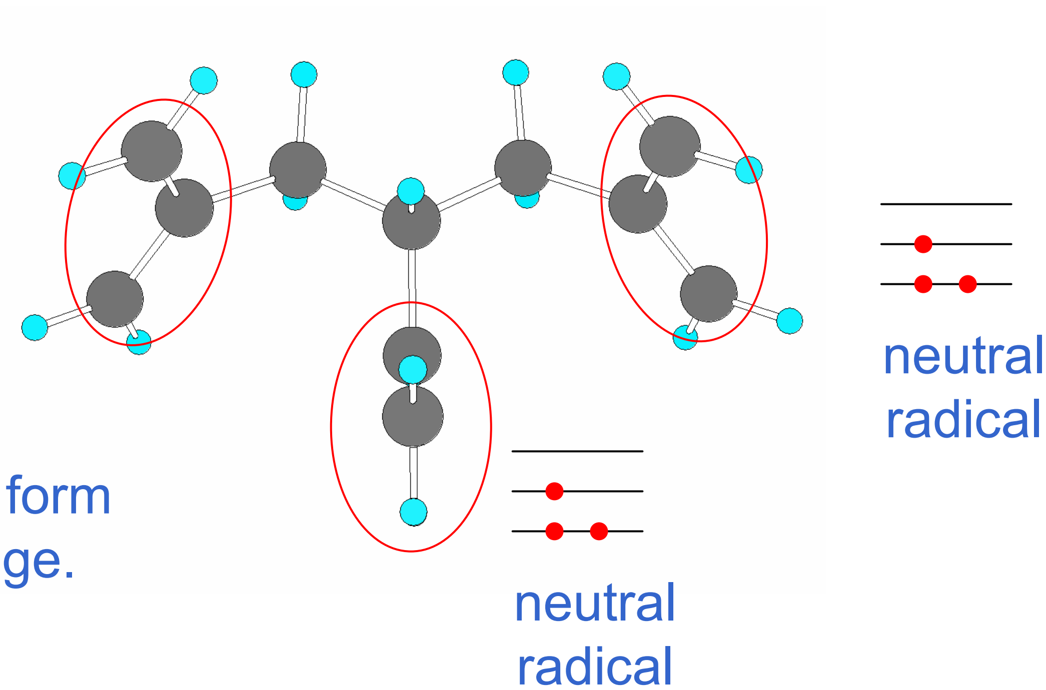
Switching molecule by a neighboring molecule



Coulomb interaction is sufficient to couple molecular states.

Molecular 3-dot cell

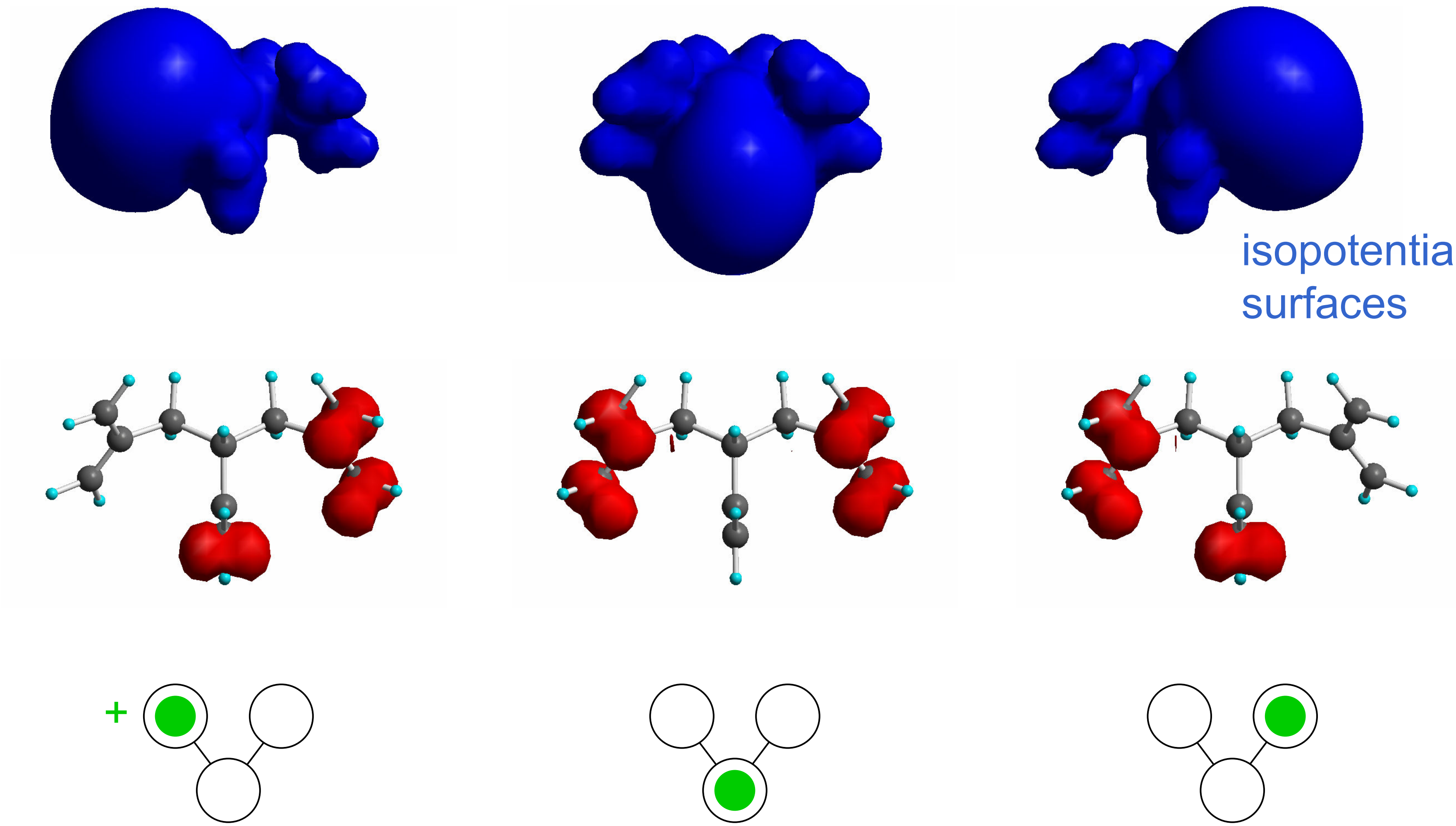




Three allyl groups form "dots" on alkyl bridge.

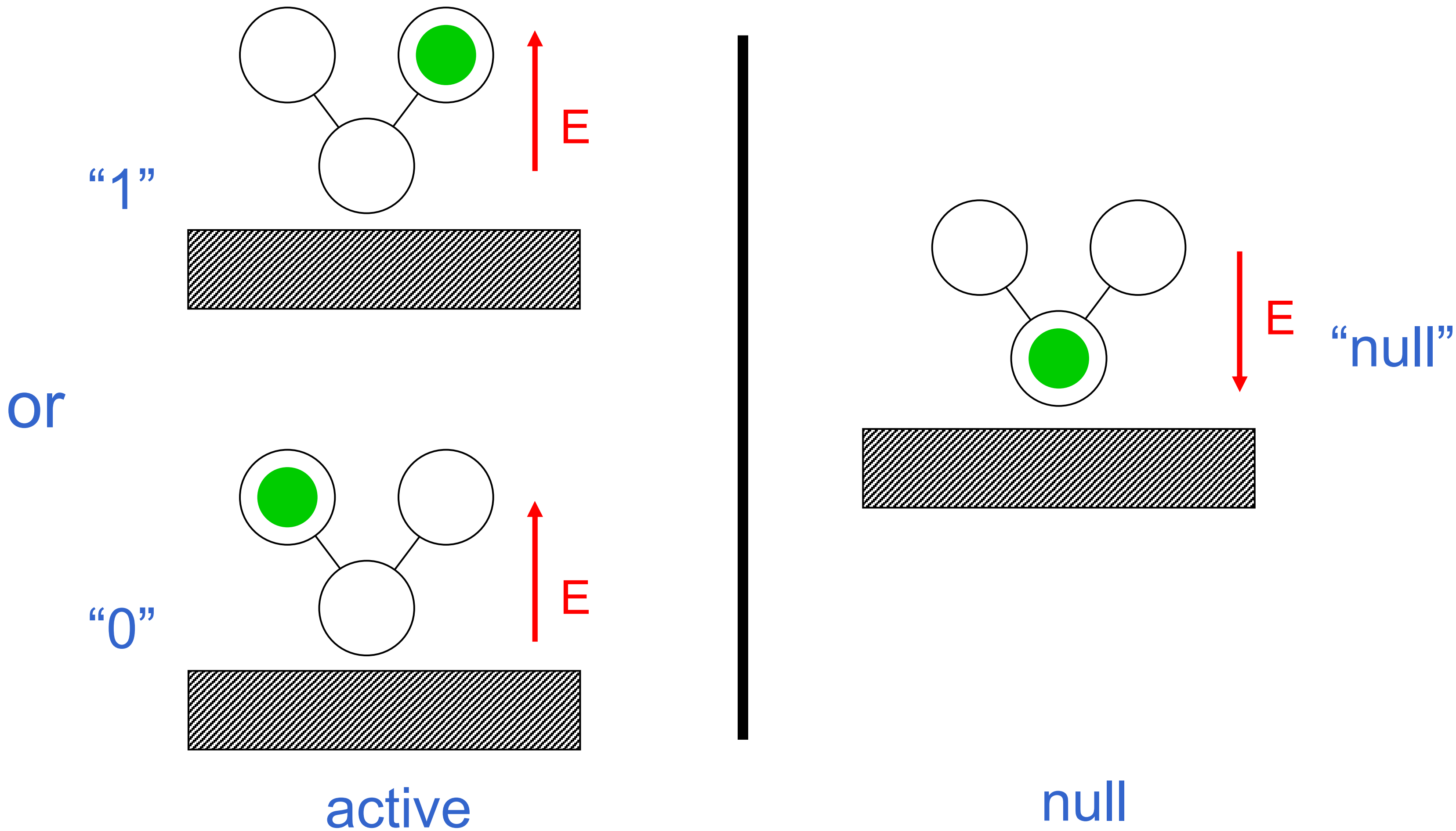
For the molecular cation, a hole occupies one of three dots.

Charge configuration represents bit



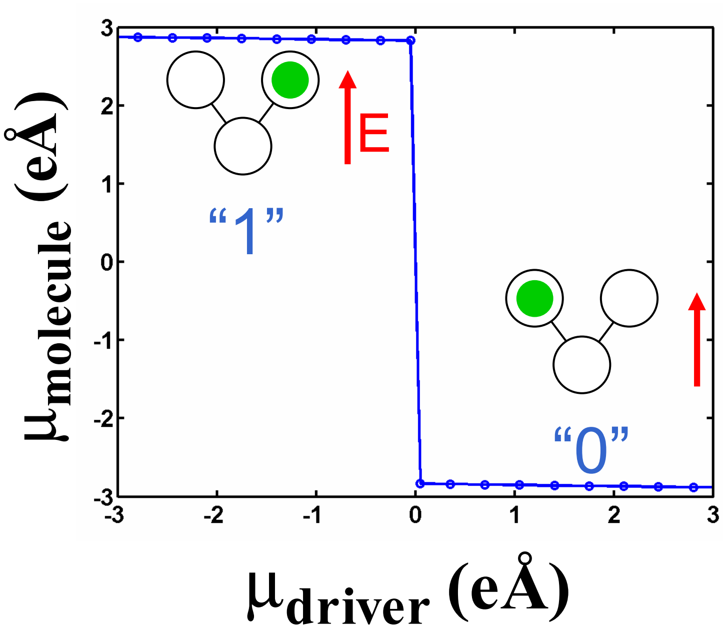
“0” “null” “1”

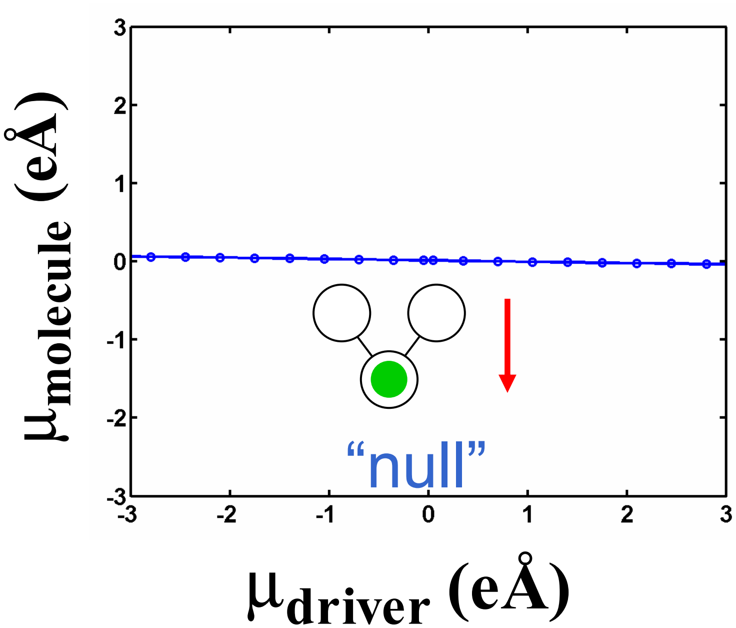
Clocking field



Use local electric field to switch molecule between active and null states.

Clocking field alters response function

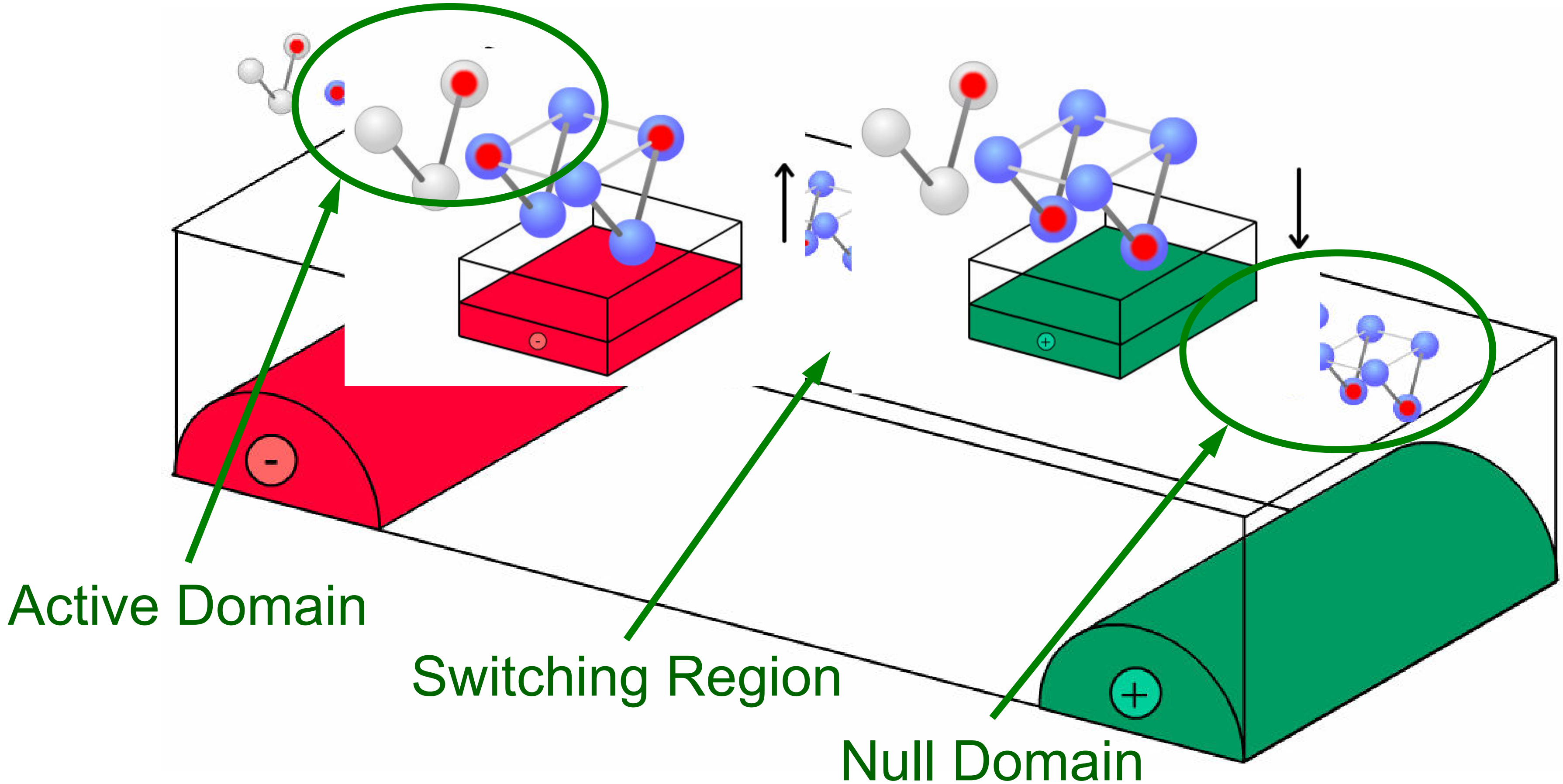




- Clocking field positive (or zero)
- Positive charge in top dots
- Cell is active – nonlinear response to input

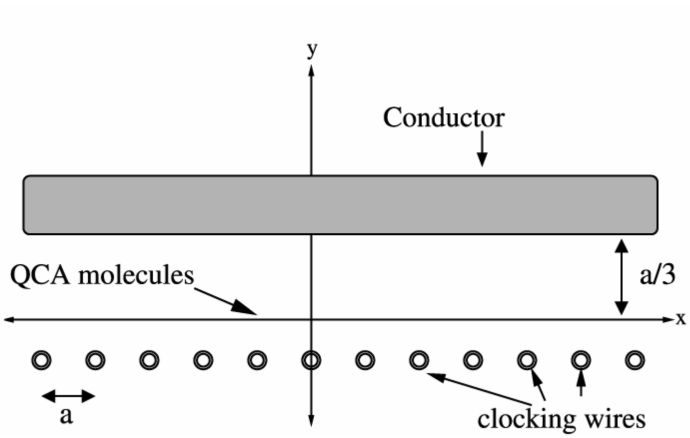
- Clocking field negative
- Positive charge in bottom dot
- Cell is inactive – no response to input

Clocked Molecular QCA

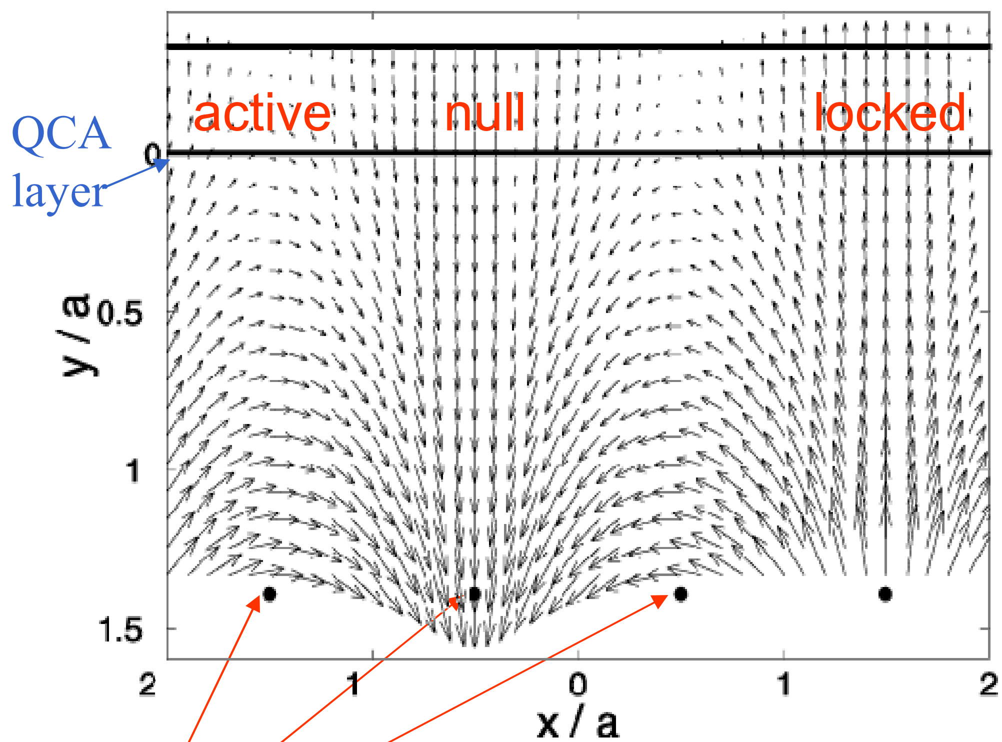


No current leads. No need to contact individual molecules.

Molecular clocking



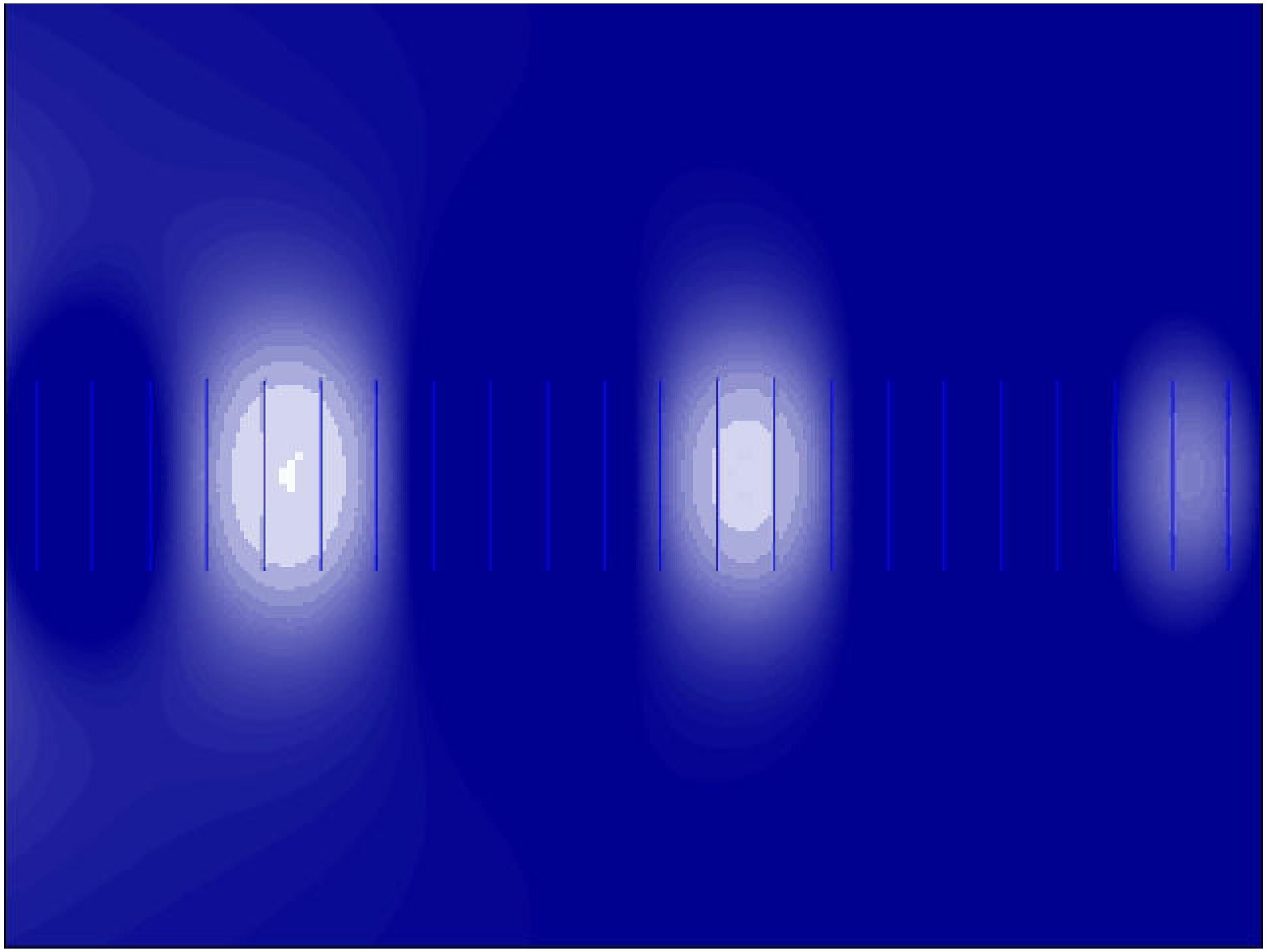
Hennessey and Lent, JVST (2001)



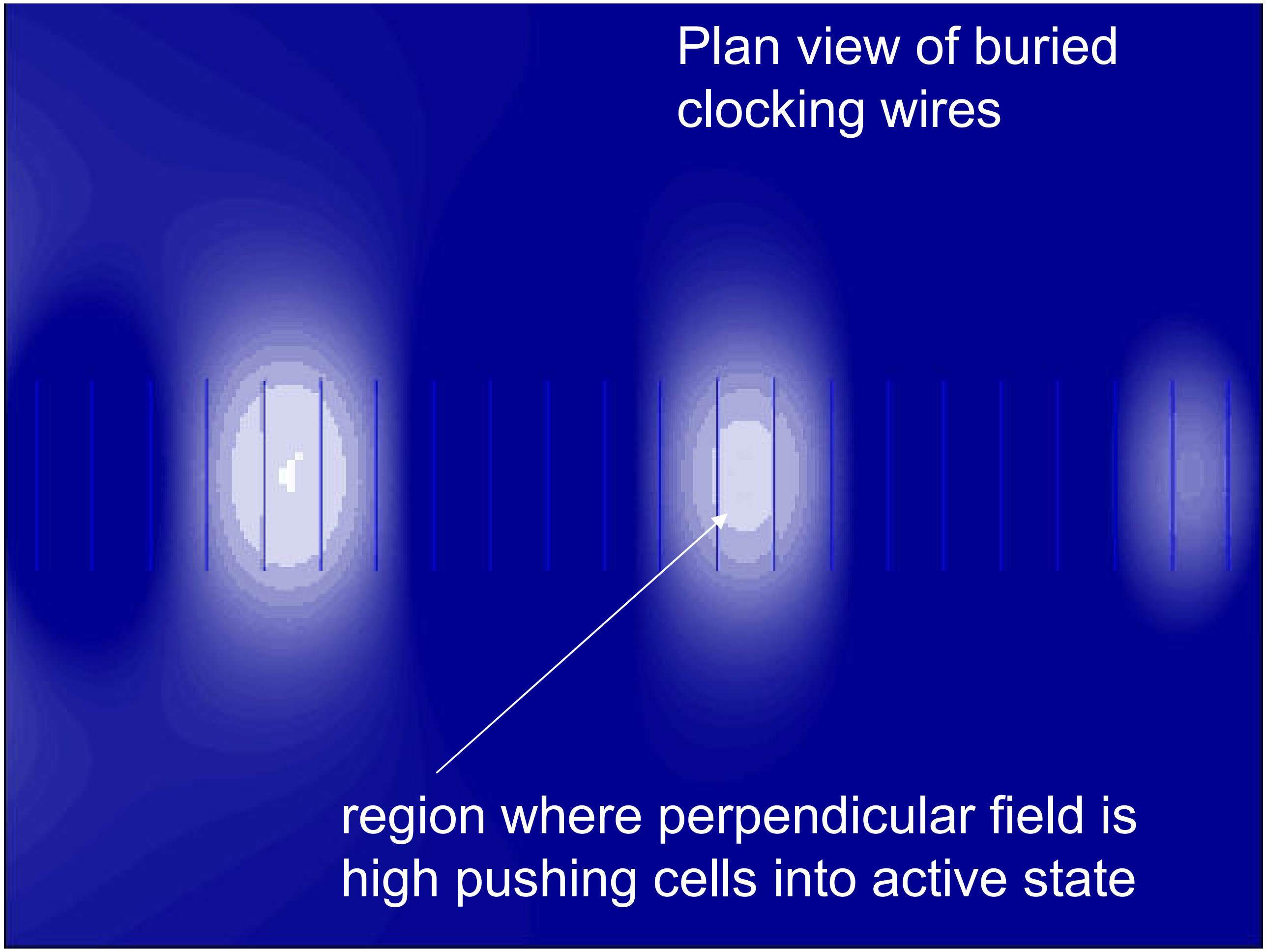
Clocking field is provided by buried wire electrodes (CMOS controlled).

Wire sizes can be 10-100 times larger than molecules.

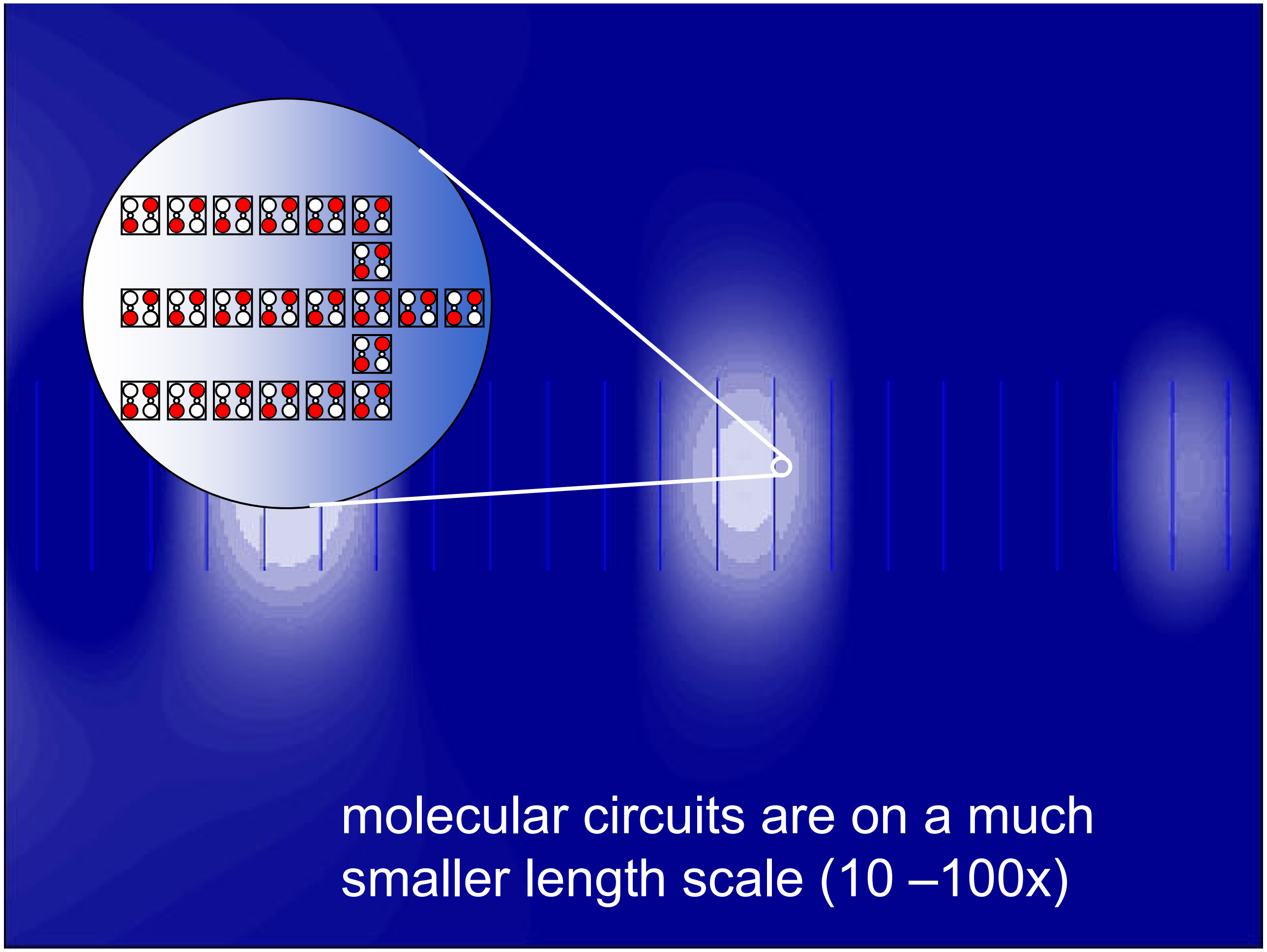
Clocking field: linear motion



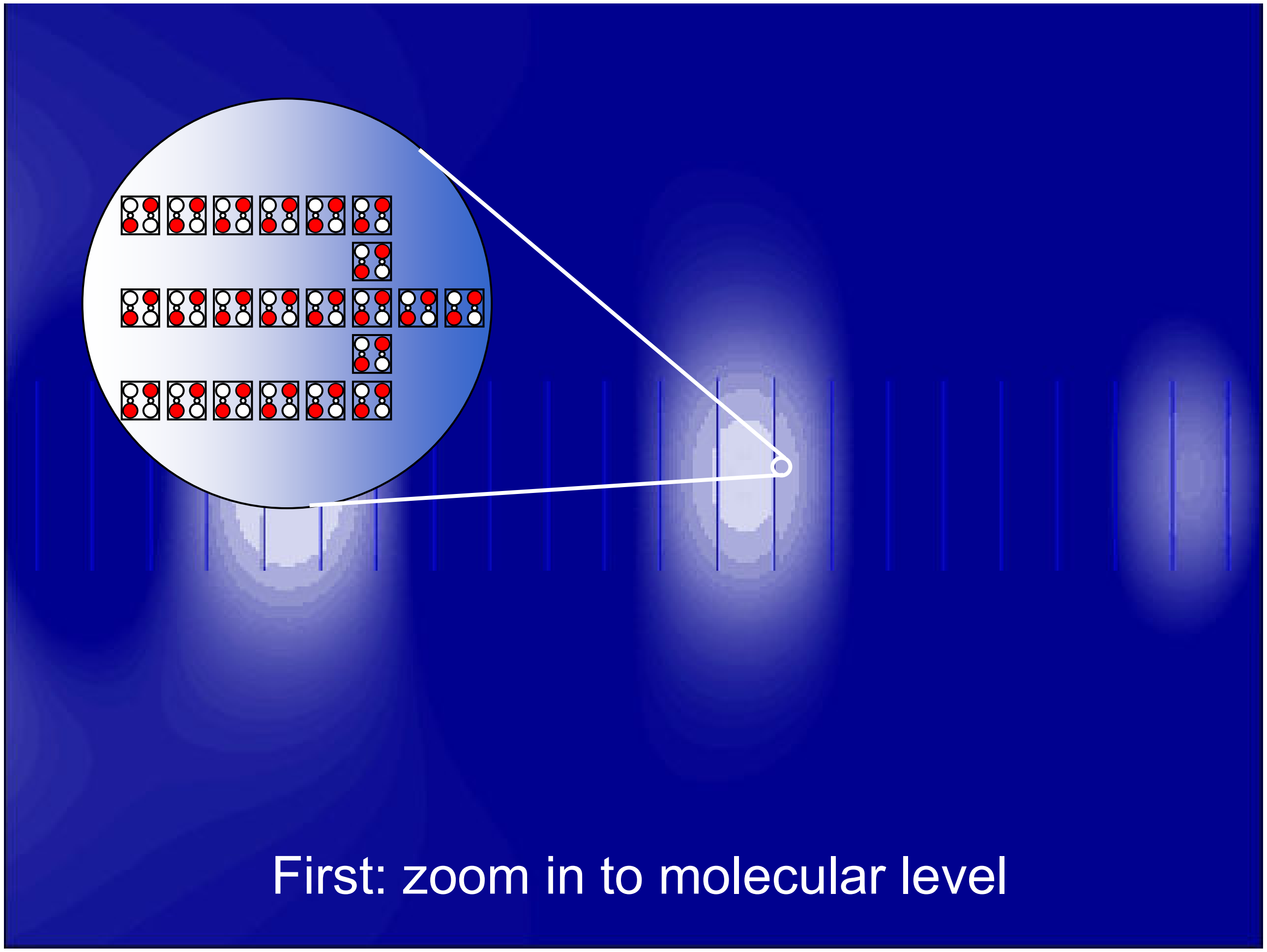
Molecular circuits and clocking wires



Molecular circuits and clocking wires



Molecular circuits and clocking wires



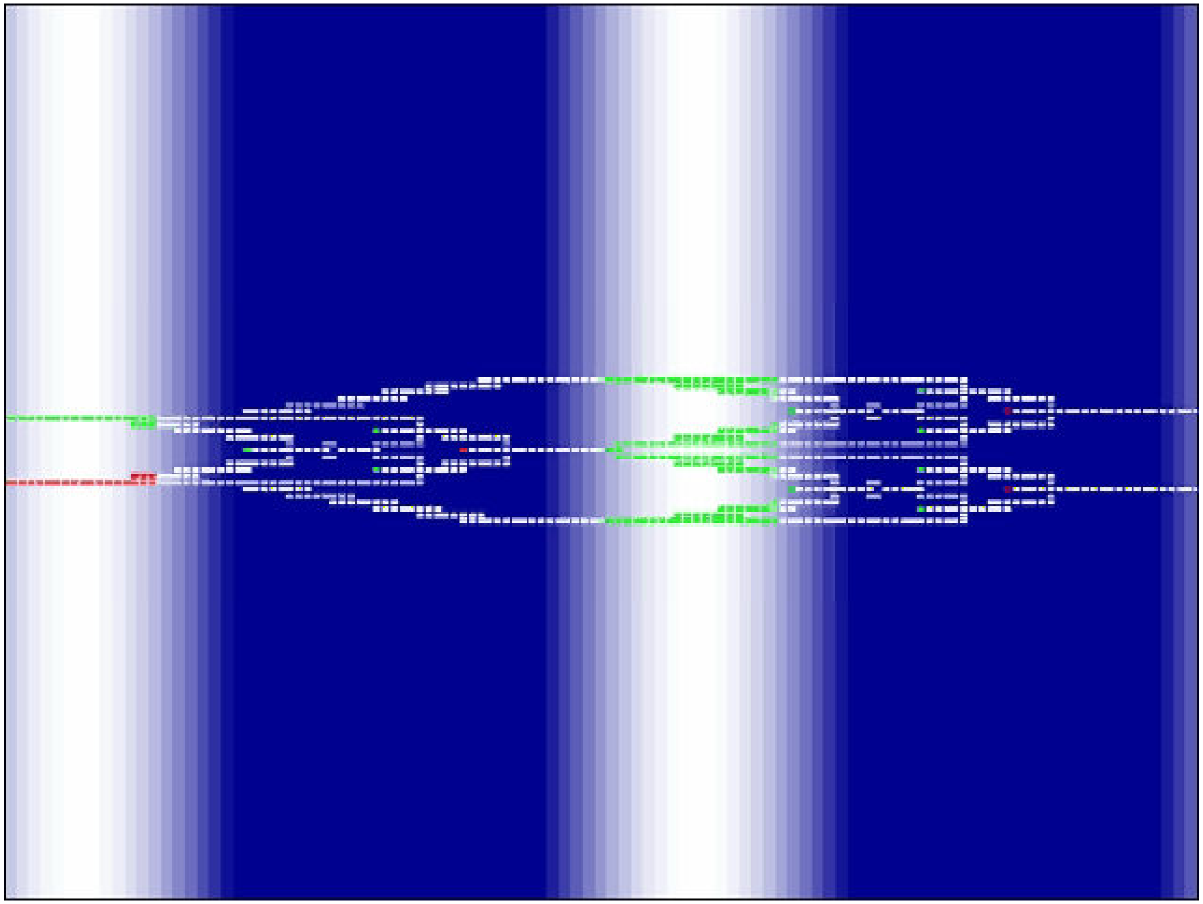
Field-clocking of QCA wire: shift-register

Computational wave: majority gate

Computational wave: adder back-end

XOR Gate

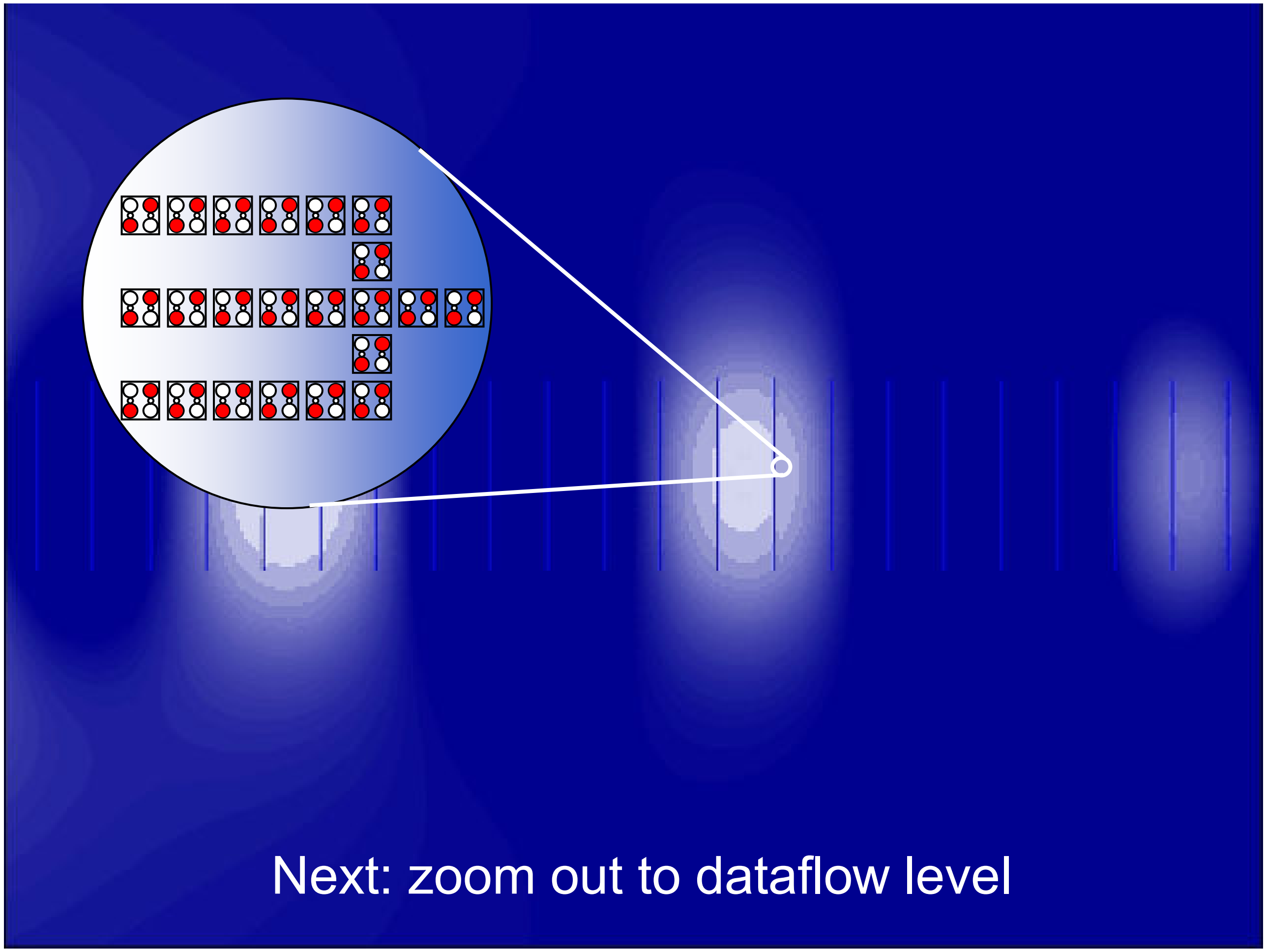
Permuter



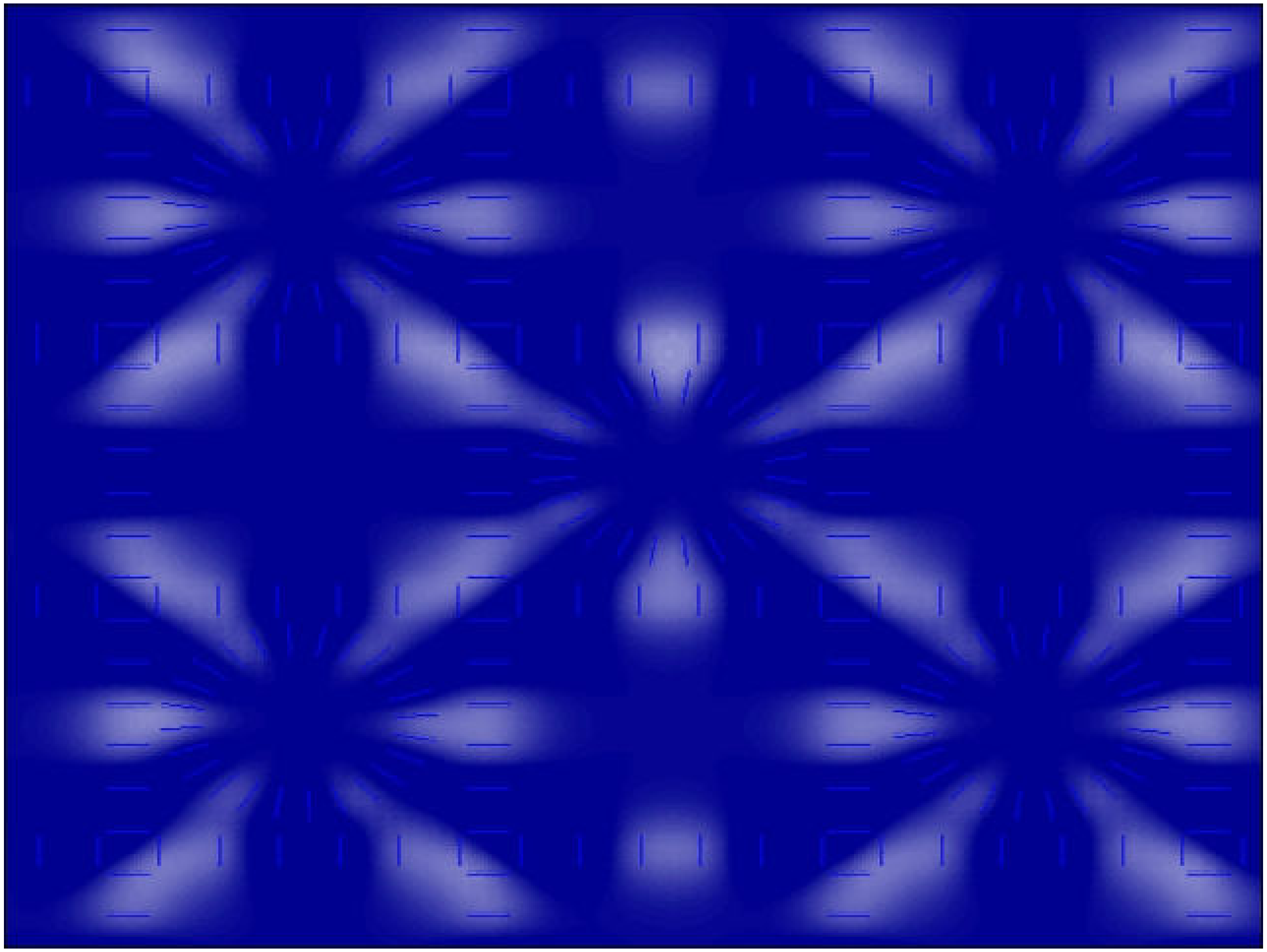
Wider QCA wires

Internal redundancy yields defect tolerance.

Molecular circuits and clocking wires



Universal floorplan



Kogge & Niemier

Outline

- Introduction
- QCA paradigm
- Implementations
  - Metal-dot QCA
  - Molecular QCA
- Energy flow in QCA
  - Power gain
  - Power dissipation and erasure
  - Bennett clocking

Power Gain in QCA Cells

- Power gain is crucial for practical devices because some energy is always lost between stages.

- Lost energy must be replaced.
  - Conventional devices – current from power supply
  - QCA devices – from the clock

- Unity power gain means replacing exactly as much energy as is lost to environment.

Power gain > 3 has been measured in metal-dot QCA.

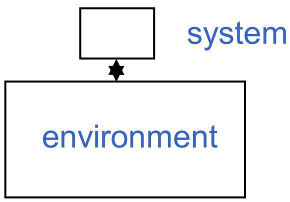
Minimum energy for computation

- Maxwell's demon (1875) – by first measuring states, could perform reversible processes to lower entropy
- Szilard (1929), Brillouin (1962): *measurement* causes $k_B T \log(2)$ dissipation per bit.
- Landauer (1961,1970): only *erasure* of information must cause dissipation of $k_B T \log(2)$ per bit.
- Bennett (1982): full computation can be done without erasure.

logical reversibility ⇔ physical reversibility

Theoretical description

Coherence vector formalism



Extract the real degrees of freedom from the density matrix

real vector $\vec{\lambda}$

$$\lambda_i = Tr(\hat{\boldsymbol{\rho}}\hat{\lambda}_i)$$

$\hat{\lambda}_i$ are the $n^2 - 1$ generators of SU(n), n=2,3

Equation of motion

$$\frac{d\vec{\lambda}}{dt} = \boldsymbol{\Omega}\vec{\lambda} + \frac{\vec{\lambda} - \vec{\lambda}_{ss}}{\tau}$$

$$\vec{\lambda}_{ss} = tr(\boldsymbol{\rho}^{eq}\hat{\lambda}_i)$$

$$\boldsymbol{\rho}^{eq} = \frac{e^{-\beta H}}{tr(e^{-\beta H})}$$

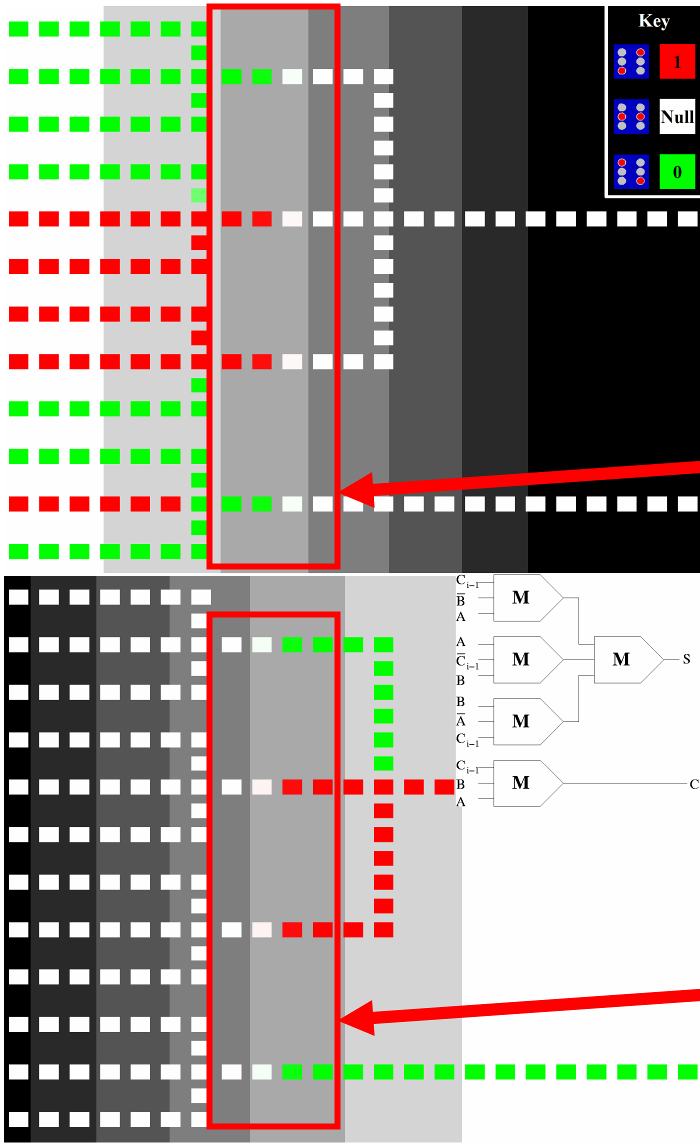
$$\boldsymbol{\Omega}_{ik} = \sum_j f_{ijk}\Gamma_j$$

$$\Gamma_j = \left(\frac{1}{\hbar}\right) tr(H\hat{\lambda}_i)$$

f_{ijk} : structure constants of SU(n)

Computational wave: adder back-end

The computational wave

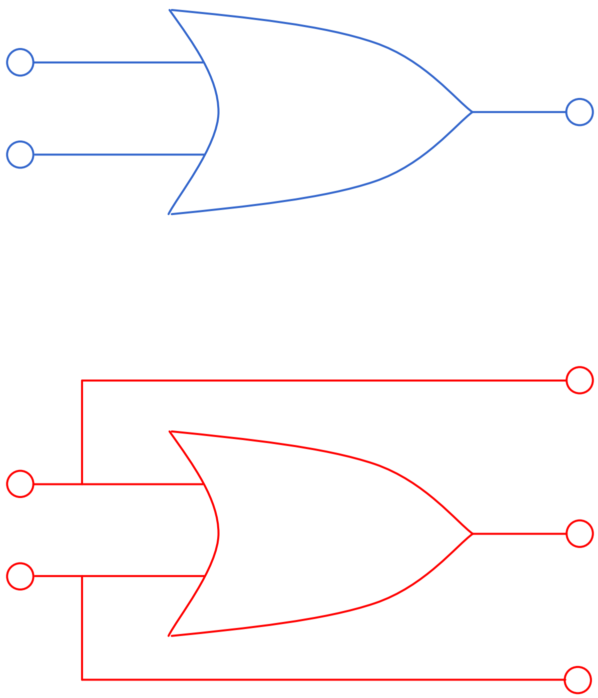


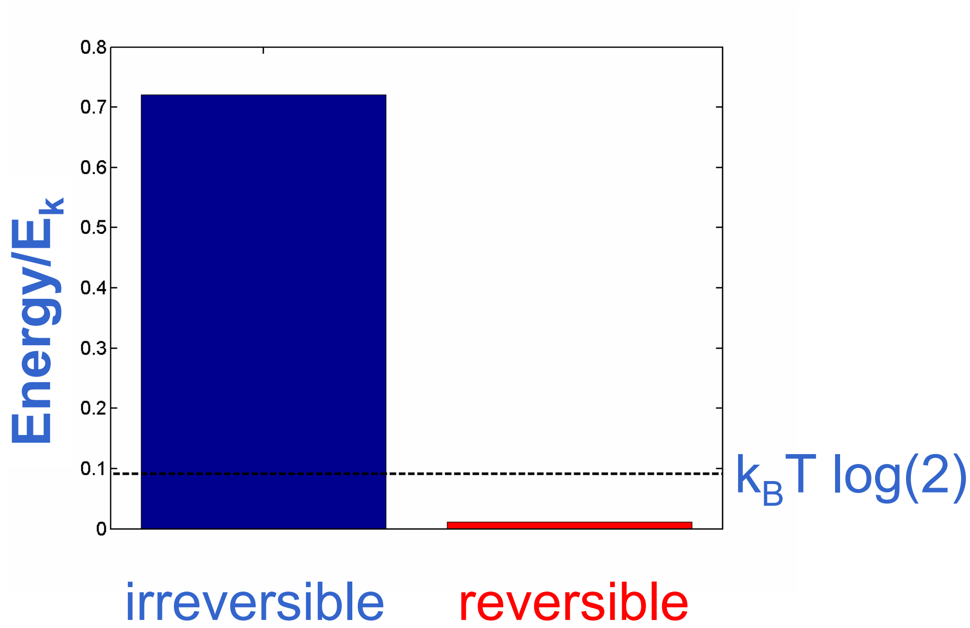
Computation happens here.

Dissipation (if any) happens here.

Landauer clocking of QCA

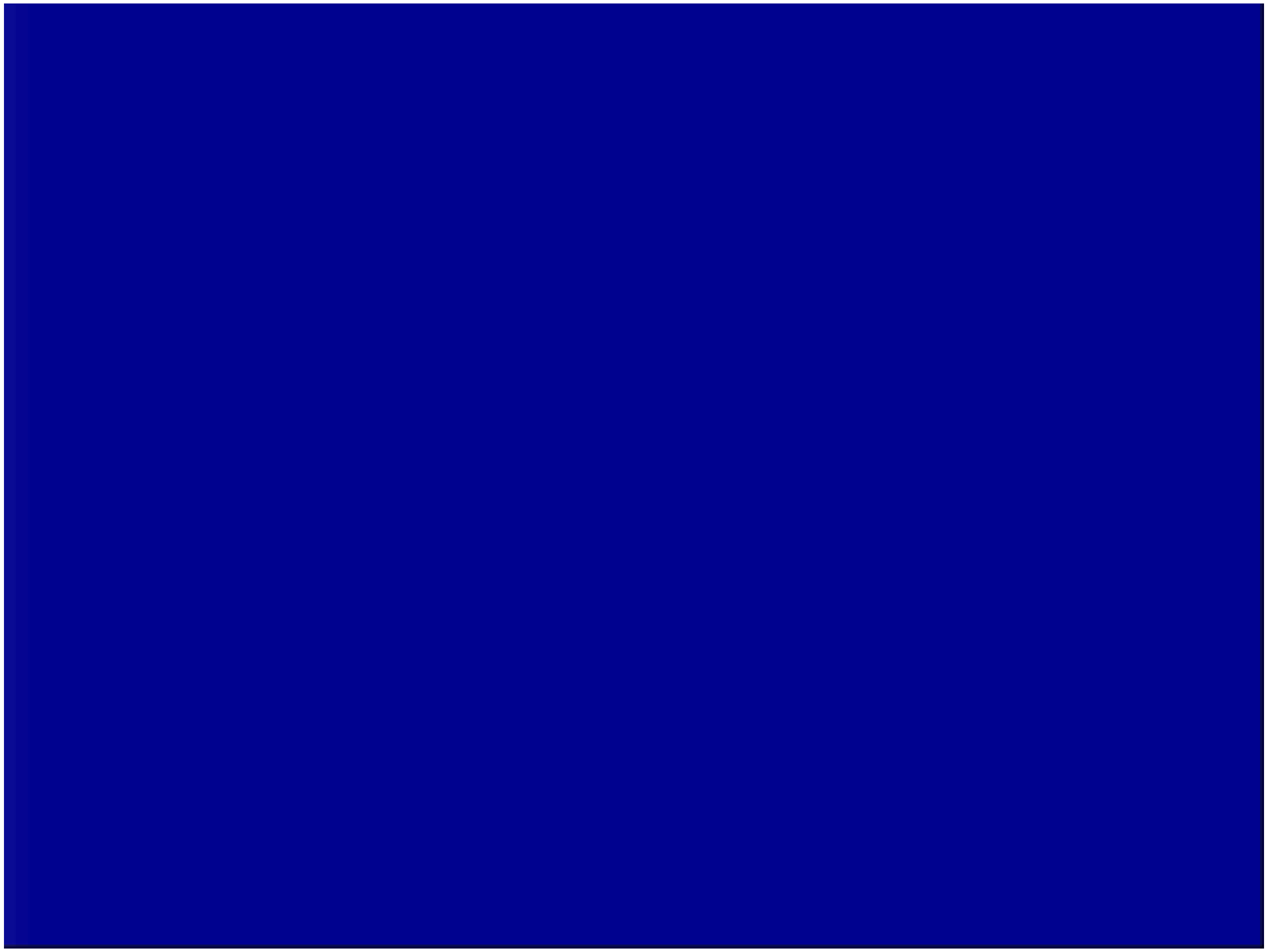
Bennett-style circuit reversibility





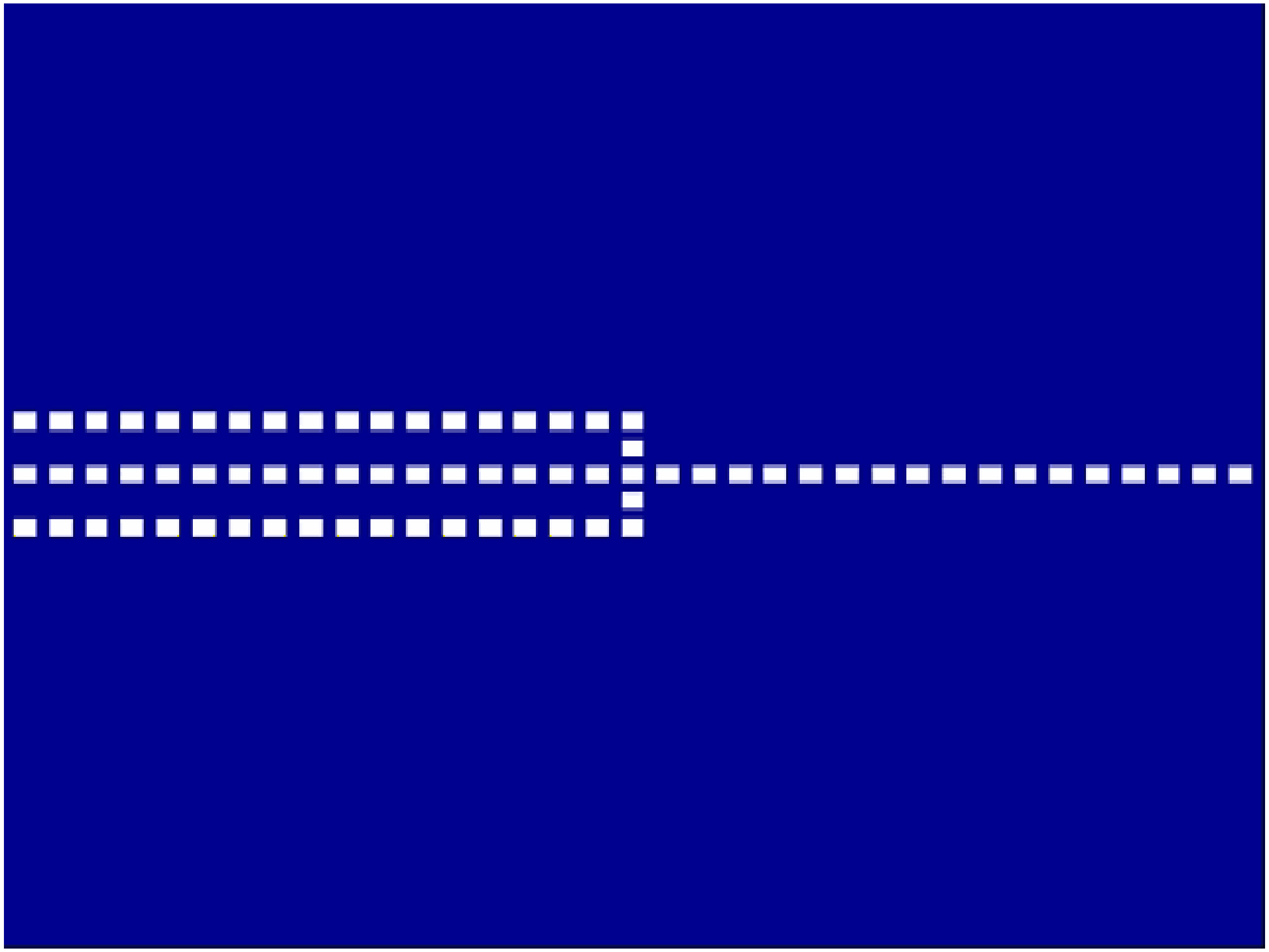
Direct time-dependent calculations shows: Logically reversible circuit can dissipate much less than $k_BT \log(2)$.

“Bennett clocking” of QCA



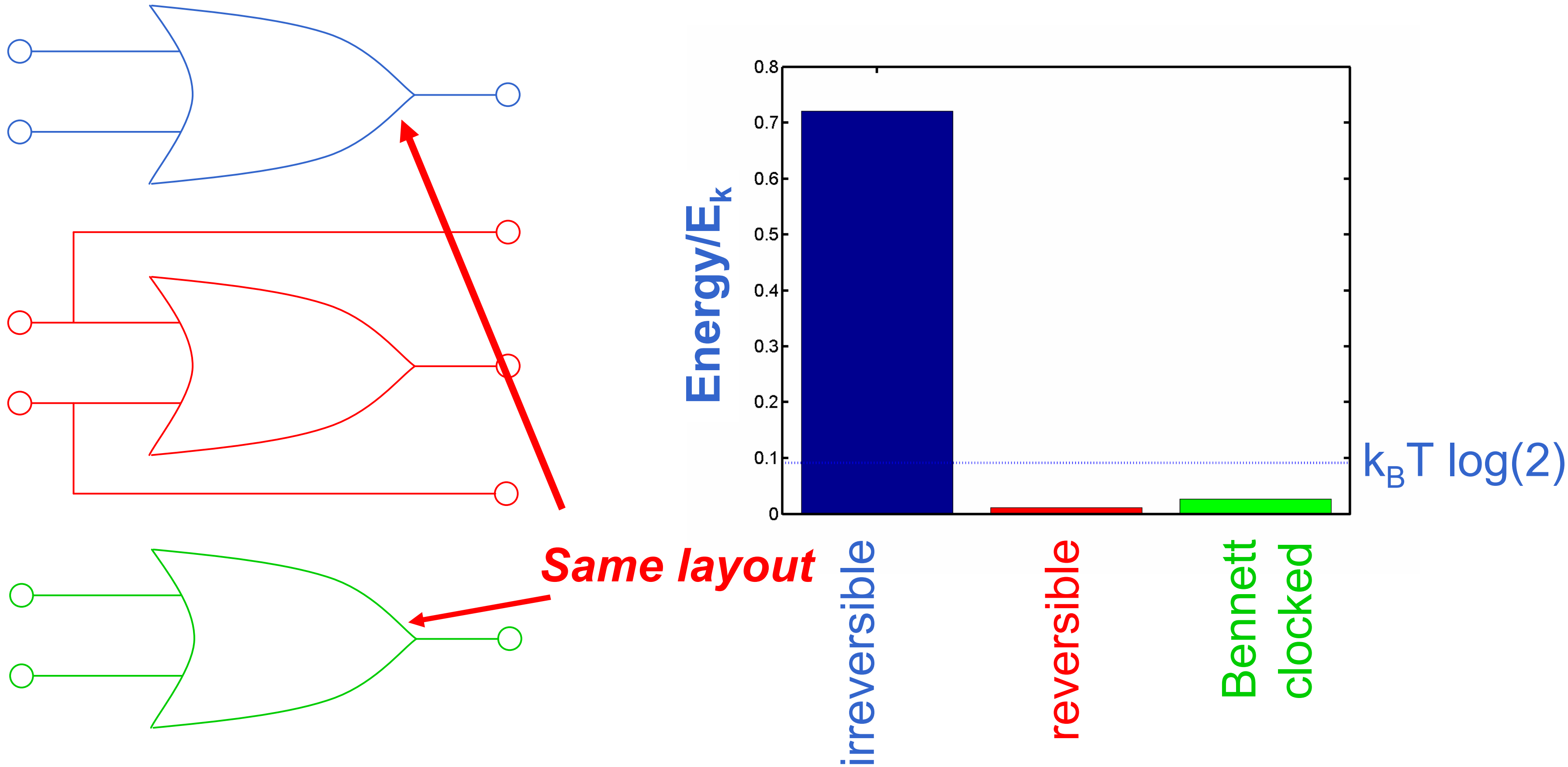
Output is used to erase intermediate results.

Bennett clocking of QCA



For QCA no change in layout is required.

QCA gate: reversible/irreversible



Direct time-dependent calculations shows: Bennett-clocked circuit can dissipate much less than $k_BT \log(2)$.

Power dissipation limits

- QCA can operate at the theoretical limits of low power dissipation.
- For regular clocking: must dissipate $k_B T \log(2)$ for each erased bit.
- For Bennett-clocking: no fundamental lower limit. Cost: half clock speed, more complicated clocking.
- Makes extreme high densities possible—clocking type is in design space.

Doesn't adiabatic mean slow?

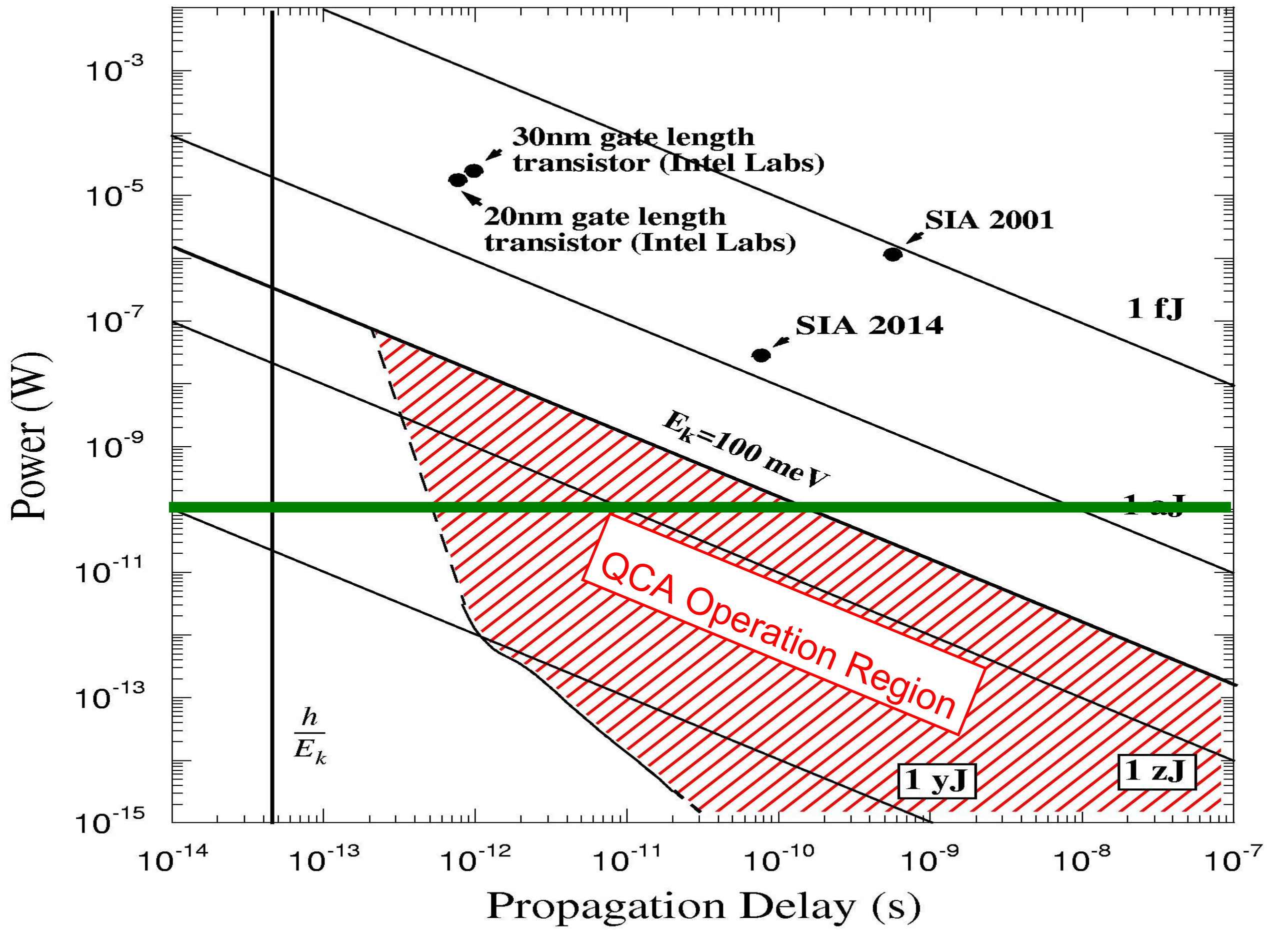
Slow compared to what?

- For conventional circuits, ω < RC

- For molecular QCA, slow compared to electron switching from one side of a molecule to the other

  $f < f_B \sim 10^{15}$ Hz $\rightarrow$ THz operation is feasible

QCA Power Dissipation



100 W/cm^2
@10^{12} devices/cm^2

QCA architectures could operate at densities 10^{12} devices/cm^2 and 100GHz without melting the chip.

Outline

- Introduction
- QCA paradigm
- Implementations
  - Metal-dot QCA
  - Molecular QCA
- Energy flow in QCA
  - Power gain
  - Power dissipation and erasure
  - Bennett clocking

Is Zettaflops computing possible?

Minimum device size: 1 nm x 1 nm

➔ 10^{14} devices/cm^2

Maximum switching speed: 10^{15} Hz

Total chip area: 10 cm x 10 cm

Maximum devices that could be switching

= $10^{14} \times 10^{15} \times 10^{2} = 10^{31}$ switches/sec

Is Zettaflops computing possible?

Downgrade density

$10^{14} \rightarrow 10^{12}$ devices/cm^2

Downgrade speed

10^{15} Hz $\rightarrow 10^{12}$ Hz

Total chip area: 10 cm x 10 cm

Gate op/flop 10^5

$\rightarrow 10^{12} \times 10^{12} \times 10^2 \times 10^{-5} = 10^{21}$ FLOPS

Possible…. but challenging

Main Points

- Quantum-dot Cellular Automata (QCA) is transistor-less approach for solving the challenges of
  - Scaling devices to molecular dimensions
  - Avoiding huge power dissipation issues
  - Power gain (lacking in crossbars)
  - Robustness against disorder

- QCA is an example of operating at the ultimate limits of low power dissipation.

- Direct calculation of the time evolution of QCA arrays illustrates the Landauer Principle. (no hand-waving required)

- QCA can be operated in a Bennett-clocking mode.
- Zettaflops operation is *conceivable*

Thank you for your attention